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NEWS 10
        AUG 15
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                 September 2003
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                PCTGEN: one FREE connect hour, per account, in
                 September 2003
                RDISCLOSURE: one FREE connect hour, per account, in
NEWS 12 AUG 15
                 September 2003
NEWS 13
        AUG 15
                 TEMA: one FREE connect hour, per account, in
                 September 2003
                Data available for download as a PDF in RDISCLOSURE
        AUG 18
NEWS 14
NEWS 15
                Simultaneous left and right truncation added to PASCAL
        AUG 18
                FROSTI and KOSMET enhanced with Simultaneous Left and Righ
NEWS 16
        AUG 18
                 Truncation
NEWS 17
        AUG 18
                Simultaneous left and right truncation added to ANABSTR
NEWS 18 SEP 22 DIPPR file reloaded
NEWS EXPRESS April 4 CURRENT WINDOWS VERSION IS V6.01a, CURRENT
              MACINTOSH VERSION IS V6.0b(ENG) AND V6.0Jb(JP),
              AND CURRENT DISCOVER FILE IS DATED 01 APRIL 2003
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L12 ANSWER 16 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN

The Diels-Alder reaction of 1,7-, 2,7-, 2,6-, and 1,6-dihydroxynaphthalene and 6-bromo-2-naphthol with maleic anhydride was investigated. All of these 2-naphthol derivs. gave exo and endo adducts except for the bromonaphthol, from which only an endo adduct was obtained. The assignment of exo or endo configuration was based on lactone formation on NaBH4 redn. (possible only from the exo isomer), comparison of NMR spectra, and in some cases dipole moment measurements. The exo-endo ratios of the formed adducts vary over a wide range. Title resolution was accomplished via the cinchonidine salts. The abs. configuration of the resolved compds. was detd. by applying the octant rule.

ACCESSION NUMBER:

1970:414534 CAPLUS

DOCUMENT NUMBER:

73:14534

TITLE:

Diels-Alder reaction. IX. Reaction of 1,7-, 2,7-,

2,6-, and 1,6-dihydroxynaphthalene and

6-bromo-2-naphthol with maleic anhydride and the resolution of some derivatives of the adducts Takeda, Kenichi; Hagishita, Sanji; Sugiura, Michi; Kitahonoki, Keizo; Ban, Isoo; Miyazaki, Sadao;

Kuriyama, Kaoru

CORPORATE SOURCE:

Shionogi Res. Lab., Shionogi and Co. Ltd., Osaka,

Japan

SOURCE:

Tetrahedron (1970), 26(6), 1435-51

CODEN: TETRAB; ISSN: 0040-4020

DOCUMENT TYPE:

Journal English

LANGUAGE:

AUTHOR (S):

29038-00-4P 29038-11-7P 29073-46-9P

29073-48-1P 29073-55-0P 29073-57-2P 29073-64-1P 29073-71-0P 29073-72-1P

29196-80-3P 29206-51-7P 31770-13-5P

31770-14-6P

RL: SPN (Synthetic preparation); PREP (Preparation)

(prepn. of)

RN 29038-00-4 CAPLUS

CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 1.alpha.,2.beta.,3.beta.,4.al pha.-tetrahydro-6-hydroxy-9-oxo-, dimethyl ester, (.+-.)- (8CI) (CA INDEX NAME)

RN 29038-11-7 CAPLUS

CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 1.alpha.,2.alpha.,3.alpha.,4. alpha.-tetrahydro-6-hydroxy-10-oxo-, dimethyl ester, (.+-.)- (8CI) (CA INDEX NAME)

RN 29073-46-9 CAPLUS

CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 1.alpha.,2.beta.,3.alpha.,4.a lpha.-tetrahydro-6-methoxy-9-oxo-, (.+-.)- (8CI) (CA INDEX NAME)

$$\begin{array}{c} \text{MeO} \\ \hline \\ \text{CO}_2\text{H} \end{array}$$

RN 29073-48-1 CAPLUS

CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 1.alpha.,2.alpha.,3.beta.,4.a lpha.-tetrahydro-6-methoxy-10-oxo-, (.+-.)- (8CI) (CA INDEX NAME)

RN 29073-55-0 CAPLUS

CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 1.alpha.,2.beta.,3.alpha.,4.a lpha.-tetrahydro-10-hydroxy-6-methoxy-, (.+-.)- (8CI) (CA INDEX NAME)

RN 29073-57-2 CAPLUS

CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 1,2,3,4-tetrahydro-6-methoxy-10-oxo-, [1R-(1.alpha.,2.beta.,3.alpha.,4.alpha.)]- (9CI) (CA INDEX NAME)

RN 29073-64-1 CAPLUS

CN Cinchonidine, (1S,2S,3S,4R)-(+)-1,2,3,4-tetrahydro-6-methoxy-9-oxo-1,4-ethanonaphthalene-2,3-dicarboxylate (1:1) (8CI) (CA INDEX NAME)

CM :

CRN 47131-85-1 CMF C15 H14 O6

CM 2

CRN 485-71-2 CMF C19 H22 N2 O

Absolute stereochemistry.

RN 29073-71-0 CAPLUS

CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 1.alpha.,2.beta.,3.beta.,4.al pha.-tetrahydro-6-methoxy-9-oxo-, dimethyl ester, (.+-.)- (8CI) (CA INDEX NAME)

RN 29073-72-1 CAPLUS

CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 1.alpha.,2.alpha.,3.alpha.,4. alpha.-tetrahydro-6-methoxy-10-oxo-, dimethyl ester, (.+-.)- (8CI) (CA INDEX NAME)

RN 29196-80-3 CAPLUS

RN 29206-51-7 CAPLUS

CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 1.alpha.,2.alpha.,3.alpha.,4. alpha.-tetrahydro-6-hydroxy-9-oxo-, dimethyl ester, (.+-.)- (8CI) (CA INDEX NAME)

RN 31770-13-5 CAPLUS

CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 1,2,3,4-tetrahydro-6-methoxy-9-oxo-, disodium salt, (1S,2S,3S,4R)-(+)- (8CI) (CA INDEX NAME)

●2 Na

RN 31770-14-6 CAPLUS

CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 1.alpha.,2.beta.,3.alpha.,4.a lpha.-tetrahydro-6-methoxy-10-oxo-, (.+-.)- (8CI) (CA INDEX NAME)

$$MeO$$
 CO_2H
 CO_2H

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STRUCTURE FILE UPDATES: 21 SEP 2003 HIGHEST RN 590345-44-1 DICTIONARY FILE UPDATES: 21 SEP 2003 HIGHEST RN 590345-44-1

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2003

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L1 STRUCTURE UPLOADED

STR

=> d query

G1 O, N

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=> s l1 SAMPLE SEARCH INITIATED 14:49:50 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 15620 TO ITERATE

6.4% PROCESSED 1000 ITERATIONS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED) SEARCH TIME: 00.00.01 FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**

PROJECTED ITERATIONS: 304922 TO 319878
PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> s l1 full FULL SEARCH INITIATED 14:49:58 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 313064 TO ITERATE

100.0% PROCESSED 313064 ITERATIONS 257 ANSWERS SEARCH TIME: 00.00.03

L3 257 SEA SSS FUL L1

=> fil caplus
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FILE COVERS 1907 - 22 Sep 2003 VOL 139 ISS 13 FILE LAST UPDATED: 21 Sep 2003 (20030921/ED)

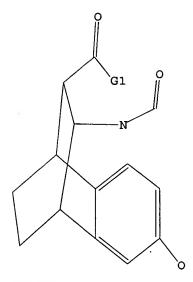
This file contains CAS Registry Numbers for easy and accurate substance identification.

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L4 STRUCTURE UPLOADED

=> d query

L4 STR



G1 O, N

Structure attributes must be viewed using STN Express query preparation.

=> s 14

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SAMPLE SEARCH INITIATED 14:51:45 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 77 TO ITERATE

100.0% PROCESSED

77 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS:

1014 TO 2066 0 TO 0

PROJECTED ANSWERS:

0 SEA SSS SAM L4

L6

L5

0 L5

=> s 14 full

REG1stRY INITIATED

Substance data SEARCH and crossover from CAS REGISTRY in progress... Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

FULL SEARCH INITIATED 14:51:52 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 1297 TO ITERATE

19 ANSWERS

100.0% PROCESSED 1297 ITERATIONS

SEARCH TIME: 00.00.01

L7 19 SEA SSS FUL L4

L8 2 L7

=> d 18 1-2 abs ibib hitstr

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Title compds. I [Rl = NR8COR9, NR8CO2R9, NR8CON(R9)2, COR9, CO2R9, CON(R9)2; R2 = OR9, N(R9)2; R3 = H, halo, OH, protected-OH, NH2, protected-NH2, alkyl, haloalkyl; R4-5 = R9, OR9, N(R9)2, N=NR9, R4, R5

together form =0, =C(R8)2, NR10 or R4-5 together with the carbon to which they are both attached form spiro carbocyclic or heterocyclic ring; R6 = H, inorg. groups having 1-8 atoms selected from boron, sulfur, phosphorous, silicon, hydrogen, and org, groups having 1-20 carbons, optionally contg. 1-4 heteroatoms selected from nitrogen, oxygen and silicon; R7 = halo, OH, protected-OH, RM2, protected-NH2, alkyl, haloalkyl; R8 = H, alkyl, aryl, heteroalkyl; R9 = H, org, groups having 1-30 carbons with the provision that two R9 groups both joined to common atom may be joined together so as to form ring with the common atom; R10

R9, OR9, N(R9)2, NHCOR9; NHCOOR9, NHCSNHR9; n is O-2; with the proviso that when R6 = H, R4-5 together form =O and R1 = CO2R2, then R2 is not OCH3] were prepd. For instance, 2,7-dihydroxynaphthalene was reacted

with maleic anhydride (1,2-dichlorobenzene/PhMe, 110.degree.C, 3 days) to afford the bicyclobenzocyclobutane adduct (16% yield). This anhydride

was reacted with 2-(trimethylsilyl)ethanol affording a 1:1 mixt. of regio isomers which was isolated as the dicyclohexylamine (DCA) salt (93% yield). The DCA salt was treated with 2M HCl permitting the isolation of the free regiolsomers which were then converted to the isopropylamine salts and crystd. affording the desired regioisomer as a 87/16 mixt. Further crystn. and liberation of the acid ester afforded II as a white solid in 30% overall yield with 98.2% purity by HPLC. Also described is

process of prepg. a combinatorial library of I from III (linker = e.g., O-CH2-C6H3-O-CH2CONH; SS = solid support; PGI = protecting group, e.g., O-ally); PGZ = protecting group, e.g., O-ABCZCETNS]. The method involves removal of PGI (PGI = O-ally), (PAI) APG/N-methylaniline) in the presence of PGZ (PGZ = OCHZCHZTMS, TBAF) and subsequent amidation with a plurality of amines; removal of PGI and amidation with a plurality of amines and 'removal of the linker (TFAaq) to liberate the corresponding bis (amides). A library of 1152 bis (amides) were prepd. in this manner. Compds. of the invention were evaluated for inhibition of apoptosis and NF. kappa.B. I are useful for inhibiting cellular events involving TNF-. alpha. and IL-8, and in the treatment of inflammation events in general.

ACCESSION NUMBER: 2002:504796 CAPLUS

DOCUMENT NUMBER: 137:78768

Freparation and use of benzobicyclobutanes as

DOCUMENT NUMBER: TITLE:

137.78768
Preparation and use of benzobicyclobutanes as inhibitors of TNF-alpha., IL-8 and for treating inflammation.
Jackson, Randy W.; Darwish, Ihab; Baughman, Ted A.; Howbert, J. Jeffry Celltech R & D, Inc., USA PCT Int. Appl., 200 pp. CODEN: PIXMO2
Patent English

INVENTOR(S):

PATENT ASSIGNEE(S):

SOURCE:

DOCUMENT TYPE: English FAMILY ACC. NUM. COUNT:

ANSWER 1 OF 2 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

. 439798-80-87 439798-81-97 439798-82-07 439798-83-17 439798-85-37 439798-86-47 439798-87-57 439798-86-67 439798-89-77 439798-97-78 439798-91-17 439798-36-77 439799-37-87 439799-36-77 439799-37-87 439799-37 4

(drug; prepn. of benzobicyclobutanes derived from Diels-Alder adduct

2,7-dihydroxynaphthalene and maleic anhydride as inhibitors of TMF-alpha., IL-8) 43798-80-8 CAPLUS 1,4-Ethanonaphthalene-2-carboxylic acid, 1,2,3,4-tetrahydro-6-hydroxy-9-oxo-3-([propoxycarbonyl]amino]-; 2-(trimethylsilyl)ethyl ester, (1R,2S,3S,4R)-rel-(SCI) (CA INDEX NAME)

Relative stereochemistry.

439798-81-9 CAPLUS
1,4-Ethanonaphthalene-2-carboxylic acid, 1,2,3,4-tetrahydro-6-hydroxy-3[([(5-methyl-3-isoxazoly1)methoxy)carbonyllamino]-9-oxo-,
2-(trimethylsily1)ethyl ester, (1R,2S,3S,4R)-rel- [9CI] (CA INDEX NAME)

Relative stereochemistry.

L8 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2003 ACS on STN PATENT INFORMATION: (Continued)

PATENT NO.			KIND DAT			APPLICATION NO.							DATE					
								-										
WO 20	WO 2002051851 WO 2002051851			2				WO 2001-US47993					20011211					
WO 20				3														
W	: AE,	AG,	AL,	AM,	AT,	ΑU,	AZ,	BA,	BB,	BG,	BR,	BY,	BZ,	CA,	CH,	CN,		
	co,	CR,	Cυ,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	ES,	FI,	GB,	GD,	GE,	GH,		
	GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	KP,	KR,	ΚZ,	LC,	LK,	LR,		
	LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	ΜX,	ΜZ,	NO,	NZ,	OM,	PH,		
	PL,	PT,	RO,	RU,	SD,	SE,	SG,	SI,	SK,	SL,	TJ,	TM,	TR.	TT,	ΤZ,	UΑ,		
	UG,	US,	UΖ,	VN,	YU,	ZA,	ZW,	AM,	ΑZ,	BY,	KG,	ΚZ,	MD,	RU,	TJ,	TM		
R	W: GH,	GM,	ΚE,	LS,	MW,	ΜZ,	SD,	SL,	SZ,	TZ,	υG,	ZM,	ZW,	AT,	ΒE,	CH,		
	CY,	DE,	DK,	ES,	FI,	FR,	GB,	GR,	IE,	IT,	LU,	MC,	NL,	PT,	SE,	TR,		
	BF,	ВJ,	CF,	CG,	CI,	CM,	GΑ,	GN,	GQ,	GW,	ML,	MR,	ΝE,	SN,	TD,	TG		
US 20	030693	A1 20030410					U.	S 20	01-1	5828		20011211						
PRIORITY A	. :				- 1	US 2	000-	2575	32P	P	2000	1222						
OTHER SOUR	CE (S):			MAR	PAT	137:	7876	8										

R SOURCE(5):

**MARPAT 137:78768

439798-63-77 439798-64-2P

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RRCT (Reactant or reagent); USES (Uses) (drug; prepn. of benzobicyclobutanes derived from Diels-Alder adduct

2,7-dihydroxynaphthalene and maleic anhydride as inhibitors of TNF-alpha., IL-8) 439798-63-7 CAPLUS 1,4-Ethanonaphthalene-2-carboxylic acid, 1,2,3,4-tetrahydro-6-hydroxy-9-ox-3-[(12-propenyloxy)carbonyl]amino]-, 2-(trimethylsilyl)ethyl ester, (1R,2S,3R,4R)-rel- (9CI) (CA INDEX NAME)

439798-84-Z MANDS 1,4-Ethanonaphthalene-2-carboxylic acid, 1,2,3,4-tetrahydro-6-hydroxy-oxo-3-[([2-propenyloxy)carbony]lamino]-, 2-(trimethylsilyl)ethyl ester (R, Z3,38,48)-rel- [961] (CA INDEX NAME)

Relative stereochemistry.

ANSWER 1 OF 2 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

439798-82-0 CAPLUS
1,4-Ethanonaphthalene-2-carboxylic acid, 1,2,3,4-tetrahydro-6-hydroxy-3[([1-methylethoxy)carbonyl]amino]-9-oxo-, 2-(trimethylsilyl)ethyl ester,
(1R,25,35,4R)-rel- (9CI) (CA INDEX NAME)

439798-83-1 CAPIUS
1,4-Ethanonaphthalene-2-carboxylic acid,
(cyclopentyloxy)carbonyl)amin
0]-1,2,3,4-tetrahydrof-6-hydroxy-9-oxo-, 2-(trimethylsilyl)ethyl ester,
(1R,2S,3S,4R)-rel- (9CI) (CA INDEX NAME)

439798-85-3 CAPLUS
1,4-Ethanonaphthalene-2-carboxylic acid, 3-[[(2,3-dihydro-1H-inden-2-yl)oxy]carbonyl]amino]-1,2,3,4-tetrahydro-6-hydroxy-9-oxo-,
2-(trimethylsilyl)ethyl ester, (1R,2S,3S,4R)-rel- (9CI) (CA INDEX NAME)

L8 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2003 ACS on STN

439798-86-4 CAPLUS
1,4-Ethanonaphthalene-2-carboxylic acid, 1,2,3,4-tetrahydro-6-hydroxy-9-oxo-3-{((2-propenylamino)carbonyl]amino)-, 2-(trimethylsilyl)ethyl ester, (1R,2S,3S,4R)-rel-(9CI) (CA INDEX NAME)

Relative stereochemistry.

439798-87-5 CAPLUS
1,4-Ethanonaphthalene-2-carboxylic acid, 1,2,3,4-tetrahydro-6-hydroxy-3[[[[2-(4-hydroxyphenyl)ethyl]amino]carbonyl]amino]-9-oxo-,
2-(trimethylsilyl)ethyl ester, (1R,2S,3S,4R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

439798-88-6 CAPLUS 43979-00-0 CREAS 1,4-Ethanonaphthalene-2-carboxylic acid, 1,2,3,4-tetrahydro-6-hydroxy-3-((4-morpholinylcarbonyl)amino)-9-00x,-2-(trimethylsilyl)ethyl ester, (1R,25,38,4R)-rel-(9CI) (CA INDEX NAME)

ANSWER 1 OF 2 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

439798-91-1 CAPLUS
1,4-Ethanonaphthalene-2-carboxylic acid, 1,2,3,4-tetrahydro-6-hydroxy-3[[[(1-naphthalenylmethyl)amino]carbonyl]amino]-9-oxo-,
2-(trimethylsilyl)ethyl ester, (1R,28,38,4R)-rel- (9CI) (CA INDEX NAME)

439799-36-7 CAPLUS
1,4-Ethanonaphthalene-2-carboxylic acid,
1,3-4-tetrahydro-6,9-dihydroxy3-[(12-propenyloxy) carbonyl]amino]-, 2-(trimethylsilyl)ethyl ester,
(1R,2S,3S,4R,9S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

439799-37-8 CAPLUS

1,4-Ethanonaphthalene-2-carboxylic acid,
:,3,4-tetrahydro-6,9-dihydroxy3-[[(2-propenyloxy)carbonyllamino]-, 2-(trimethylsilyl)ethyl ester,
(lR,2S,3R,4R,9S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

L8 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2003 ACS on STN Relative stereochemistry. (Continued)

439798-89-7 CAPLUS
1,4-Ethanonaphthalene-2-carboxylic acid, 3-{{{1,1-dimethylethyl|amino|-1,2,3,4-tetrahydro-6-hydroxy-9-oxo-,2-{trimethylsilyl)ethyl|ester, {1R,2S,3S,4R}-rel- {9CI} (CA INDEX NAME)

439798-90-0 CAPLUS
1,4-Ethanonaphthalene-2-carboxylic acid, 3-{{{{(2,4-

dimethoxyphenyl)methyl]amino]carbonyl]amino]-1,2,3,4-tetrahydro-6-hydroxy9-oxo-, 2-(trimethylsilyl)ethyl ester, (1R,2S,3S,4R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

ANSWER 1 OF 2 CAPLUS COPYRIGHT 2003 ACS on STN

439799-80-1 CAPLUS
1,4-Ethanonaphthalene-2-carboxylic acid,
3,4-tetrahydro-6,9-dihydroxy:
3-{((2-propenyloxy)carbonyl]amino}-, 2-(trimethylsilyl)ethyl ester,
(1R,2S,3S,4R,9R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

439800-25-6 CAPLUS
1,4-Ethanonaphthalene-2-carboxylic acid, 1,2,3,4-tetrahydro-6-hydroxy-9-oxo-3-[[pentylamino]carbonyl]amino]-, 2-(trimethylsilyl)ethyl ester, [IR,2S,3S,4R)-rel- [9CI] (CA INDEX NAME)

```
L8 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2003 ACS on STN
AB A novel series of TNF-alpha. inhibitors based on a benzobicyclooctane scaffold was reported. The compds. displayed good potency in inhibiting TNF-alpha. induced apoptosis and NF kappa B activation. Addnl., they were selective for TNF-alpha. as they did not inhibit apoptosis induced by sol. Fas ligand. The compds. described here can act as leads for future medicinal chem. efforts and may also be useful tools for elucidating the TNF-alpha. signaling pathway.

ACCESSION NUMBER: 2002:21239 CAPLUS
DOCUMENT NUMBER: 137:288467
TITLE: Benzobicyclooctanes as novel inhibitors of TNF-alpha.
signaling
```

signaling Jackson, Randy W.; Gelinas, Richard; Baughman, Ted

AUTHOR(S):

Cox, Thomas: Howbert, J. Jeffry; Kucera, Kristin A.; Latham, John A.; Ramsdell, Fred; Singh, Devinder; Darwish, Ihab S. Department of Chemical Genomics, Celltech R&D, Inc., Bothell, WA, 98021, USA Bioorganic & Medicinal Chemistry Letters (2002), 12(7), 1093-1097 CODEN: BMCLES; ISSN: 0960-894X Elsevier Science Ltd. Journal

CORPORATE SOURCE:

CODEN: EMCLE8; ISSN: 0960-894X

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

T 48008-82-0P 468086-83-1P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
(Uses)
(benzobicyclocotanes as novel inhibitors of TNF-.alpha. signaling)

RN 468086-82-0 CAPLUS

C 1,4-Ethanonaphthalene-2-carboxylic acid, 3-[[[[1,1'-biphenyl]-4ylmethoxylcarbonyl]amino]-1,2,3,4-tetrahydro-6-hydroxy-9-oxo-,
2-(trimethylsilyl)ethyl ester, (1R,2S,3S,4R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

468086-83-1 CAPLUS
1,4-Ethanonaphthalene-2-carboxylic acid, 1,2,3,4-tetrahydro-6-hydroxy-9-oxo-3-[[[(3-pyridinylmethyl)amino]carbonyl]amino]-, 2(trimethylsilyl)ethyl ester, (1R,2S,3S,4R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

L8 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

REFERENCE COUNT:

20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR

RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

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COST IN U.S. DOLLARS

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CA SUBSCRIBER PRICE

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STRUCTURE FILE UPDATES: 21 SEP 2003 HIGHEST RN 590345-44-1 DICTIONARY FILE UPDATES: 21 SEP 2003 HIGHEST RN 590345-44-1

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2003

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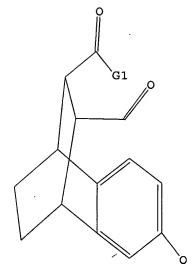
Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details: http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

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L9 STRUCTURE UPLOADED

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Structure attributes must be viewed using STN Express query preparation.

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SAMPLE SEARCH INITIATED 14:55:45 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 411 TO ITERATE

100.0% PROCESSED 411 ITERATIONS 8 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

COMPLETE BATCH

PROJECTED ITERATIONS: 7004 TO 9436 8 TO 329

PROJECTED ANSWERS:

L10 8 SEA SSS SAM L9

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FULL SEARCH INITIATED 14:55:49 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 8166 TO ITERATE

100.0% PROCESSED 8166 ITERATIONS 229 ANSWERS

SEARCH TIME: 00.00.01

L11 229 SEA SSS FUL L9

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FILE 'CAPLUS' ENTERED AT 14:55:53 ON 22 SEP 2003

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FILE COVERS 1907 - 22 Sep 2003 VOL 139 ISS 13 FILE LAST UPDATED: 21 Sep 2003 (20030921/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l11 L12 16 L11

=> d 112 1-16 abs ibib hitstr

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Title compds. I [Rl = NRBCOR9, NRBCO2R9, NRBCON(R9)2, COR9, CO2R9, COM(R9)2; R2 = OR9, N(R9)2; R3 = H, halo, OH, protected-OH, NH2, protected-NH2, alkyl, haloalkyl; R4-5 = R9, OR9, N(R9)2, N=NR9, R4, R5

together form =0, =C(RB)2, NR10 or R4-5 together with the carbon to which they are both attached form spiro carbocyclic or heterocyclic ring; R6 = R, inorg, groups having 1-8 atoms selected from boron, sulfur, phosphorous, silicon, hydrogen, and org, groups having 1-20 carbons, optionally contg. 1-4 heteroatoms selected from nitrogen, oxygen and silicon; R7 = halo, OH, protected-OH, NR2, protected-HN2, alkyl, haloalkyl; R8 = H, alkyl, aryl, heteroalkyl; R9 = H, org, groups having 1-30 carbons with the provision that two R9 groups both joined to common atom may be joined together so as to form ring with the common atom; R10

R9, OR9, N(R9)2, NHCOR9; NHCOOR9, NHCSNHR9; n is 0-2; with the proviso that when R6 = H, R4-5 together form =0 and R1 = CO2R2, then R2 is not OCH3] were prepd. For instance, 2,7-dihydroxynaphthalene was reacted

maleic anhydride (1,2-dichlorobenzene/PhMe, 110.degree.C, 3 days) to afford the bicyclobenzocyclobutane adduct (16% yield). This anhydride

was reacted with 2-(trimethylsilyl)ethanol affording a 1:1 mixt. of regio isomers which was isolated as the dicyclohexylamine (DCA) salt (93% yield). The DCA salt was treated with 2M HCI permitting the isolation of the free regioisomers which were then converted to the isopropylamine salts and crystd. affording the desired regioisomer as a 87/16 mixt. Further crystn. and liberation of the acid ester afforded II as a white solid in 30% overall yield with 98.2% purity by HPLC. Also described is

solid in 30% overall yield with 98.2% purity by HPIC. Also described is a process of prepg. a combinatorial library of I from III [linker = e.g., O-CH2-CGH5-O-CH2CONH; SS = solid support; PG1 = protecting group, e.g., O-ally1; PG2 = protecting group, e.g., CR2CHZTMS]. The method involves removal of PG1 [PG1 = O-ally1, (Ph3)4Pd/N-methylaniline) in the presence of PG2 (PG2 = OCH2CHZTMS, TBAF) and subsequent amidation with a plurality of amines; removal of PG2 and amidation with a plurality of amines; nemoval of the linker (TFAnq) to liberate the corresponding bis (amides). A library of 1152 bis (smides) were prepd. in this manner. Compds. of the invention were evaluated for inhibition of apoptosis and NF kappa.B. I are useful for inhibiting cellular events involving TNF-alpha. and IL-8, and in the treatment of inflammation events in general.

ACCESSION NUMBER: 2002:504796 CAPPLUS
DOCUMENT NUMBER: 137:78768

INVENTOR(S): Jackson, Randy W.; Darwish, Ihab; Baughman, Ted A.; Howbert, J. Jeffry
PATENT ASSIGNEE(S): Celltech R & D, Inc., USA
SOURCE: PCT Int. Appl., 200 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent
LANGUAGE: PCT Int. Appl., 200 pp.
CODEN: PIXXD2

PATENT ASSIGNEE(S): CODEN: PIXXD2

PATENT ASSIGNEE(S): PCT Int. Appl., 200 pp.

L12 ANSWER 1 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN INDEX NAME) (Continued)

Relative stereochemistry.

439798-65-9 CAPLUS 1,4-Ethanonaphthalene-2-carboxylic acid, 1,2,3,4-tetrahydro-3-[[methyl[2-

-2-{[(2,4,6-trimethoxyphenyl)methyl]amino]ethyl]amino]carbonyl}-10-oxo-7-[[4-[(2-propenyloxy)carbonyl)phenyl]methoxyl-, 2-(trimethylsilyl)ethyl eater, (1R,2s,3R,48)-rel- (9C) (CA INDEX NAME)

Relative stereochemistry.

PAGE 1-A

L12 ANSWER 1 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN PATENT INFORMATION: (Continued)

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			LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NO,	NZ,	OM,	PH,		
			PL,	PΤ,	RO,	RU,	SD,	SE,	SG,	SI,	SK,	SL,	TJ,	TM,	TR,	TT,	TZ,	UA,		
															MD,					
		RW:	GH,	GΜ,	ΚE,	LS,	MW,	ΜZ,	SD,	SL,	SZ,	TZ,	υG,	ZM,	ZW,	ΑŤ,	BE,	CH,		
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	OTHER S	OURCE	(S):			MAR	PAT	137:	7876	8										

R SOURCE(S): MARRAT 137:78768
A39799-73-2DP, combinatorial library of amide derivs.
RL: CPN (Combinatorial preparation); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); CMBI (Combinatorial study); PREP (Preparation); USES (Uses) (drug; prepn. of benzobicyclobutanes derived from Diels-Alder adduct

2,7-dihydroxynaphthalene and maleic anhydride as inhibitors of TNF-.alpha., IL-8)
439799-73-2 CAPLUS
1,4-Ethanonaphthalene-2,3-dicarboxamide, 1,2,3,4-tetrahydro-6-hydroxy-9-oxo-, (1R,23,38,48)-rel- (9CI) (CA INDEX NAME)

419798-64-8P 439798-65-9P 439798-66-0P 439798-67-1P 439798-68-2P 439798-72-8P 439798-78-4P 439798-79-5P 439798-92-2P 439798-78-4P 439798-79-67 439798-79-69 439799-84-5P 439799-84-5P 439799-86-79 439799-86-79 79-79-79-79

2,7-dihydroxynaphthalene and maleic anhydride as inhibitors of TTF-.alpha., IL-8) 439798-64-8 CAPLUS 1,4-Ethanonaphthalene-2-carboxylic acid, 1,2,3,4-tetrahydro-7-hydroxy-3-

[[methyl[2-oxo-2-[{{2,4,6-trimethoxyphenyl}methyl]amino]ethyl]amino]carbon yl]-10-oxo-, 2-(trimethylsilyl)ethyl ester, (1R,2S,3R,4S)-rel- (9CI) (CA

L12 ANSWER 1 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

PAGE 1-B

439798-66-0 CAPLUS
Benzoic acid, 4-[[{[1R,2s,3R,4s}-3-[(dipentylamino)carbonyl]-1,2,3,4-

439798-67-1 CAPLUS
Benzoic acid, 4-{{{(1R,2S,3R,4S)-3-{(dipentylamino)carbonyl}-1,2,3,4-

Relative stereochemistry.

RN 439798-68-2 CAPLUS
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid,
1,2,3,4-tetrahydro-6-hydroxy9-oxo-, 3-[(2,4-dimethoxyphenyl)methyl] 2-[2-(trimethylsilyl)ethyl]

ester, (1R,2s,3s,4s)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

L12 ANSWER 1 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

439798-92-2 CAPLUS
1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 1,2,3,4-tetrahydro-9-oxo-6[(4-[(2-propenyloxy)carbonyl]phenyl]methoxy]-, 3-propyl
2-[2-(crimethylsilyl)ethyl] ester, (1R,2S,3S,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

439799-40-3 CAPLUS

1,4-Ethanonaphthalene-2,3-dicarboxylic acid,
3,4-tetrahydro-6-hydroxy9-[[(4-methylphenyl)methyl]amino]-, 3-propyl 2-[2-(trimethylsilyl)ethyl]
ester, (1R,2S,3S,4S,9R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 439799-41-4 CAPLUS
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid,
1,2,3,4-tetrahydro-6-hydroxy9-(methylamino)-,3-propyl 2-(2-(trimethylsilyl)ethyl] ester,
(1R,2S,3S,4S,9R)-rel- (9CI) (CA INDEX NAME)

L12 ANSWER 1 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN

RN 439798-72-8 CAPLUS
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid,
1,2,3,4-tetrahydro-6-hydroxy9-oxo-, 3-propyl 2-{2-(trimethylsily1)ethyl} ester, {1r,2s,3s,4s}-rel(9CI) (CA INDEX NAME)

(Continued)

Relative stereochemistry.

RN 439798-78-4 CAPLUS
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid,
1,2,3,4-tetrahydro-6-hydroxy9-oxo-, 3-(2-propenyl) 2-[2-(trimethylsilyl)ethyl] ester,
(1R,2S,3S,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

439798-79-5 CAPLUS
1,4-Ethanonaphthalene-2-carboxylic acid, 3-{azidocarbonyl}-1,2,3,4-tetrahydro-6-hydroxy-9-oxo-, 2-(trimethylsilyl)ethyl ester, (lR,2S,3S,4S)-rel-(9CI) (CA INDEX NAME)

Relative stereochemistry.

L12 ANSWER 1 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN Relative stereochemistry. (Continued)

439799-45-8 CAPLUS
1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 9-(acetylmethylamino)-6-(acetyloxy)-1,2,3,4-tetrahydro-, 3-propyl 2-(2-(trimethylsilyl)ethyl)ester, (1R,2S,3S,4S,9R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 439799-84-5 CAPLUS
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid,
1,2,3,4-tetrahydro-6-hydroxy9-[{(4-methyl)henyl)methyl]amino]-, 3-propyl 2-[2-(trimethylsilyl)ethyl]
ester, (1R,2S,3S,4S,9S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

439799-86-7 CAPLUS

1,4-Ethanonaphthalene-2,3-dicarboxylic acid,
3,4-tetrahydro-6-hydroxy9-(methylamino)-, 3-propyl 2-{2-(trimethylsilyl)ethyl} ester,
(1R,2S,3S,4S,9S)-rel- (9CI) (CA INDEX NAME)

L12 ANSWER 1 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN

439799-90-3 CAPLUS
1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 9-(acetylmethylamino)-6(acetyloxy)-1,2,3,4-tetrahydro-, 3-propyl 2-[2-(trimethylsilyl)ethyl)
ester, (IR,2S,3S,4S,9S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

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364778-16-5P 439798-61-5P 439798-62-6P
439798-63-3P 439798-61-5P 439798-62-6P
439798-63-3P 439798-70-6P 439798-71-7P
439798-73-9P 439798-74-0P 439798-73-3P
439798-76-2P 439798-95-5P 439798-93-3P
439798-90-6P 439798-91-6P 439798-92-6P
439798-00-5P 439798-01-6P 439798-02-7P
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439798-10-1P 439799-14-1P 439799-13-2P
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L12 ANSWER 1 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

439798-69-3 CAPLUS
1,4-Ethanonaphthalene-2,3-dicarboxylic acid,
3,4-tetrahydro-6-methoxy9-oxo-, 3-[{2,4-dimethoxyphenyl}methyl] 2-[2-(trimethylsilyl)ethyl] ester, (1R,2s,3s,4s)-rel- (9CI) (CA INDEX NAME)

439798-70-6 CAPLUS 1,4-Ethanonaphthalene-2-carboxylic acid, 3-[[[(2,4-

dimethoxyphenyl]methyl]amino]carbonyl]-1,2,3,4-tetrahydro-6-methoxy-9-oxo-, 2-(trimethylsilyl)ethyl ester, (1R,2S,3S,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

439798-71-7 CAPLUS
1,4-Ethanonaphthalene-2-carboxylic acid, 3-[(dipentylamino)carbonyl]1,2,3,4-ctrahydro-6-hydroxy-9-oxo-, 2-(trimethylsilyl)ethyl ester,
(1R,2S,3S,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

L12 ANSWER 1 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)
438800-24-5P 439800-26-7P 439800-27-8P
439800-28-9P 439919-18-3P 439919-19-4P
RL: PAC (Pharmacological activity): SPN (Synthetic preparation): THU
(Therapeutic use): BIOL (Biological study): PREP (Preparation): USES (drug; prepn. of benzobicyclobutanes derived from Diels-Alder adduct

of
2,7-dihydroxynaphthalene and maleic anhydride as inhibitors of
TNF-alpha., IL-8)
RN 364778-16-5 CAPLUS
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 6-[2-(1,1-dimethylethoxy)-2-oxoethoxy]-1,2,3,4-tetrahydro-9-oxo-, 3-propyl
2-[2-(trimethylsityl)ethyl]
ester, '(1R,2S,3S,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 439798-61-5 CAPLUS CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 1,2,3,4-tetrahydro-6-hydroxy-9-oxo-, 2-[2-(trimethylsily1)ethy1) ester, (1R,2S,3R,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 439798-62-6 CAPLUS
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid,
1,2,3,4-tetrahydro-6-hydroxy9-oxo-, 3-[2-(trimethylsilyl)ethyl] ester, (1R,2S,3R,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

L12 ANSWER 1 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

RN 439798-73-9 CAPLUS
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid,
1,2,3,4-tetrahydro-6-hydroxy9-oxo-, 3-[2-(cyclohexyloxy)ethyl] 2-[2-(trimethylsilyl)ethyl] ester,
(1R,2S,3S,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 439798-74-0 CAPLUS
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid,
1,2,3,4-tetrahydro-6-hydroxy9-oxo-, 3-(2-(3-pytidiny))ethyl) 2-(2-(trimethylsilyl)ethyl) ester,
(IR,28,38,48)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

439798-75-1 CAPLUS

L12 ANSWER 1 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN (Continued) .

CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid,
1,2,3,4-tetrahydro-6-hydroxy9-oxor, 3-[(3-fluorophenyl)methyl] 2-[2-(trimethylsilyl)ethyl] ester,
(1R,2S,3S,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 439798-76-2 CAPLUS
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid,
1,2,3,4-tetrahydro-6-hydroxy9-oxor, 3-[2-[1-pyrrolidinyl]ethyl] 2-[2-(trimethylsilyl)ethyl] ester,
{1R,2S,3S,4S}-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 439798-77-3 CAPLUS
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid,
1,2,3,4-tetrahydro-6-hydroxy9-oxo-, 3-dodecyl 2-[2-(trimethylsilyl)ethyl] ester, (1R,2S,3S,4S)-rel(9CI) (CA INDEX NAME)

Relative stereochemistry.

L12 ANSWER 1 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

439798-96-6 CAPLUS
1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 1,2,3,4-tetrahydro-6-{2-{2-naphthaleny}}ethoxy]-9-oxo-, 3-propyl 2-{2-(trimethylsilyl)ethyl] ester, (1R,2S,3S,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

439798-97-7 CAPLUS
1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 6-[(3-fluorophenyl)methoxyl-1,2,3,4-tetrahydro-9-oxo-, 3-propyl 2-[2-(trimethylsilyl)ethyl] ester, (1R,2S,3S,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

Relative stereochemistry.

L12 ANSWER 1 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

RN 439798-93-3 CAPLUS
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 6-{2-(diethylamino}-2-oxoethoxy]-1,2,3,4-tetrahydro-9-oxo-, 3-propyl
2-{2-(trimethylailyl)ethyl]
ester, (1R,2S,3S,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

439798-94-4 CAPLUS
1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 1,2,3,4-tetrahydro-6-[(4-nitrophenyl)methoxyl-9-oxo-, 3-propyl 2-[2-(trimethylsilyl)ethyl] ester, (lR,2S,3S,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 439798-95-5 CAPLUS
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 6-{[1,1'-biphenyl}-4-ylmethoxy]-1,2,3,4-tetrahydro-3-oxo-, 3-propyl
2-{2-{trimethylsilyl=thyl}
ester, (1R,2S,3S,4S}-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

L12 ANSWER 1 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

RN 439798-99-9 CAPLUS
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid,
1,2,3,4-tetrahydro-9-oxo-6-[2[2-pyridinyl)ethoxy]-, 3-propyl 2-[2-(trimethylsilyl)ethyl] ester,
[R,28,38,48]-rel- (9C1) (CA INDEX NAME)

Relative stereochemistry.

439799-00-5 CAPLUS
1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 1,2,3,4-tetrahydro-6-(2-methoxyethoxyl)-9-oxo-, 3-propyl 2-[2-(trimethylsilyl)ethyl] ester, (1R,2S,3S,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

439799-01-6 CAPLUS
1.4-Ethenonaphthalene-2,3-dicarboxylic acid, 6-(cyclopentyloxy)-1,2,3,4-tetrahydro-9-oxo-,3-propyl 2-[2-(trimethylsilyl)ethyl) ester, (1R,2S,3S,4S)-rel- (9CI) (CA INDEX NAME)

439799-02-7 CAPLUS
1,4=Sthanonaphthalene-2,3-dicarboxylic acid, 6-{3-cyanopropoxy}-1,2,3,4-tetrahydro-9-oxo-,3-propyl 2-[2-(trimethylsilyl)ethyl] ester,
[1R,2S,3S,4S]-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

439799-03-8 CAPLUS
1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 1,2,3,4-tetrahydro-6-[(5-methyl-3-isoxazolyl)methoxy]-9-oxo-, 3-propyl 2-[2-(trimethylsilyl)ethyl]ester, (1R,2S,3S,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 439799-04-9 CAPLUS
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid,
6-ethoxy-1,2,3,4-eterahydro-9oxo-, 3-propyl 2-[2-(trimethylsilyl)ethyl] ester, (1R,2S,3S,4S)-rel-(CA INDEX NAME)

Relative stereochemistry.

L12 ANSWER 1 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

RN 439799-08-3 CAPLUS
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid,
1,2,3,4-tetrahydro-9-oxo-6-{2pyridinylmethoxyl-, 3-propyl 2-{2-(trimethylsilyl)ethyl} ester,
{1R,2S,3S,4S}-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

439799-09-4 CAPLUS

1,4-Ethanonaphthalene-2,3-dicarboxylic acid,
[(dimethoxyphosphinylloxy]1,2,3,4-tetrahydro-9-oxo-, 3-propyl 2-[2-(trimethylsilyl)ethyl] ester,
(1R,2S,3S,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

439799-11-8 CAPLUS
1,4-Ethanonaphthalene-2,3-dicarboxylic acid,
2,3,4-tetrahydro-6-hydroxy9-(methyhydrazono)-, 3-propyl 2-{2-(trimethylsilyl)ethyl} ester,
{1R,2S,3S,4S,9E}-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry. Double bond geometry as shown.

L12 ANSWER 1 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

RN 439799-05-0 CAPLUS
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid,
1,2,3,4-tetrahydro-6-methoxy9-oxo-, 3-propyl 2-[2-(trimethylsilyl)ethyl] ester, (1R,2S,3S,4S)-rel(9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 439799-06-1 CAPLUS
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid,
1,2,3,4-tetrahydro-9-oxo-6-[2propenjloxy]-,3-propyl 2-[2-(trimethylsily1)ethyl] ester,
(1R,2S,3S,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 439799-07-2 CAPLUS
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid,
1,2,3,4-tetrahydro-9-oxo-6-{3pyridinylmethoxyl-, 3-propyl 2-[2-(trimethylsilyl)ethyl) ester,
(1R,2S,3S,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

L12 ANSWER 1 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

439799-12-9 CAPLUS
1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 9-(cyclohexylhydrazono)1,2,3,4-tetrahydro-6-hydroxy-, 3-propyl 2-[2-(trimethylsilyl)ethyl] (1R,2S,3S,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry. Double bond geometry unknown.

RN 439799-13-0 CAPLUS
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid,
9-((2-bromophenyl)) Nydrazono]1,2,3,4-tetrahydro-6-hydroxy-, 3-propyl 2-(2-(trimethylsilyl)ethyl)
ester,
(lR,2s,3s,4s)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry. Double bond geometry unknown.

RN 439799-14-1 CAPLUS
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid,
9-(dimethylhydrazono)-1,2,3,4tetrahydro-6-hydroxy-,3-propyl 2-[2-(trimethylsilyl)ethyl] ester,
(1R,2S,3S,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry. Double bond geometry unknown

RN 439799-15-2 CAPLUS
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid,
1,2,3,4-tetrahydro-6-hydroxy9-[(2-hydroxyethyl)hydrazono]-, 3-propyl 2-[2-(trimethylsilyl)ethyl]
ester, (1R,2S,3S,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry unknown.

439799-16-3 CAPLUS
1,4=Ethanonaphthalene-2,3-dicarboxylic acid, 9[(aminothloxomethyl)hydrazono]-1,2,3,4-tetrahydro-6-hydroxy-, 3-propyl
2-[2-(trimethylsilyl)ethyl) ester, (1R,2S,3S,4S)-rel- (9CI) (CA INDEX
NAME)

Relative stereochemistry. Double bond geometry unknown.

L12 ANSWER 1 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN Relative stereochemistry. Double bond geometry as shown. (Continued)

RN 439799-20-9 CAPLUS
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid,
1,2,3,4-tetrahydro-6-hydroxy9-[(phenylaulfonyl)hydrazono]-, 3-propyl 2-[2-(trimethylsilyl)ethyl]
ester, (1R,2S,3S,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry unknown.

439799-21-0 CAPLUS
1,4-Ethanonaphthalene-2,3-dicarboxylic acid,
3,4-tetrahydro-6-hydroxy9-[[(4-methoxyphenyl)sulfonyl]hydrazono]-, 3-propyl 2-[2(trimethylsilyl)ethyl] ester, (1R,2S,3S,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry unknown.

439799-22-1 CAPLUS
1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 9-{acetylhydrazono}-1,2,3,4-tetrahydro-6-hydroxy-, 3-propyl 2-[2-(trimethylsilyl)ethyl) ester,

L12 ANSWER 1 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

RN 439799-17-4 CAPLUS
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid,
1,2,3,4-tetrahydro-6-hydroxy9-[[(methylamino)thioxomethyl]hydrazono]-, 3-propyl 2-[2(trimethylsilyl)ethyl] ester, (1R,2S,3S,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry unknown.

439799-18-5 CAPLUS

1,4-Ethanonaphthalene-2,3-dicarboxylic acid,
3,4-tetrahydro-6-hydroxy9-(methylphenylhydrazono)-, 3-propyl 2-[2-(trimethylsilyl)ethyl] ester,
(1R,2S,3S,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry. Double bond geometry unknown

RN 439799-19-6 CAPLUS
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid,
1,2,3,4-tetrahydro-6-hydroxy9-[(methylsulfonyl)hydrazono]-, 3-propyl 2-[2-(trimethylsilyl)ethyl]
ester, (1R,2S,3S,4S,92)-rel- (9CI) (CA INDEX NAME)

L12 ANSWER 1 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN (1R,2S,3S,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry unknown

RN 439799-23-2 CAPLUS
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid,
1,2,3,4-tetrahydro-6-hydroxy9-(hydroxyimino)-, 3-propyl 2-[2-(trimethylsilyl)ethyl] ester,
(1R,2S,3S,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry unknown.

439799-24-3 CAPLUS
1,4-Ethanonaphthalene-2,3-dicarboxylic acid,
3,4-tetrahydro-6-hydroxy9-(methoxylmino)-,3-propyl 2-[2-(trimethylsilyl)ethyl] ester,
(1R,2S,3S,4S,9E)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown

L12 ANSWER 1 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN (Continue N 439799-25-4 CAPLUS COPYRIGHT 2003 ACS on STN (Continue N 149799-25-4 CAPLUS COPYRIGHT 2003 ACS on STN (Continue N 1,2,3,4-tetrahydro-6-hydroxy-9-(phenoxyimino)-, 3-propyl 2-{2-(trimethylsilyl)ethyl) ester, {1R,2S,3S,4S}-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry unknown.

RN 439799-26-5 CAPLUS
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid,
1,2,3,4-tertanylor-6-hydroxy9-[(phenylmethoxy)imino]-, 3-propyl 2-[2-(trimethylsilyl)ethyl] ester,
[RR,2S,35,45,92]-rel- (9C1) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.

RN 439799-27-6 CAPLUS 1,4-Ethanonaphthalene-2,3-dicarboxylio'acid,
1,2,3,4-tetraphydro-6-hydroxy9-[((4-nitrophenyl)methoxylimino]-, 3-propyl 2-[2-(trimethylsilyl)ethyl]
ester, (1R,2S,3S,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry unknown.

L12 ANSWER 1 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN

439799-31-2 CAPLUS
1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 9-[[(4fluorophenyl)methoxy]imino]-1,2,3,4-tetrahydro-6-hydroxy-, 3-propyl
2-[2-(trimethylsilyl)ethyl) ester, (IR,2S,3S,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry unknown

RN 439799-32-3 CAPLUS
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid,
1,2,3,4-tetrahydro-6-hydroxy9-[(2-phenoxyethoxylimino]-, 3-propyl 2-[2-(trimethylsilyl)ethyl] ester,
{1R,2S,3S,4S}-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry unknown.

RN 439799-33-4 CAPLUS
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid,
1,2,3,4-tetrahydro-6-hydroxy9-[(2-propenyloxy)imino]-, 3-propyl 2-(2-(trimethylsilyl)ethyl) ester,
(1R,2S,3S,4S)-rel- (9CI) (CA INDEX NAME)

L12 ANSWER 1 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)
439799-28-7 CAPLUS
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 9-{{5-chloro-1,2,3-thiadiazo1-4-yl]methoxylimino]-1,2,3,4-tetrahydro-6-hydroxy-, 3-propyl
2-[2-{trimethylsilylethyl} ester, (1R,2S,3S,4S)-rel- (9CI) (CA INDEX

Relative stereochemistry.
Double bond geometry unknown.

439799-29-8 CAPLUS
1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 9-[[(3-fluorophenyl)methoxy]imino]-1,2,3,4-tetrahydro-6-hydroxy-, 3-propyl
2-[2-(trimethylsilyl)ethyl] ester, (1R,2S,3S,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry unknown.

RN 439799-30-1 CAPLUS
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid,
1,2,3,4-tetrahydro-6-hydroxy9-[[2-oxo-2-(4-phenyl-1-piperazinyl)ethoxy]imino]-, 3-propyl
2-[2-(trimethylsilyl)ethyl] ester, (1R,2S,3S,4S,9E)-rel- (9CI) (CA INDEX

Relative stereochemistry.
Double bond geometry as shown.

L12 ANSWER 1 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN Relative stereochemistry. Double bond geometry unknown. (Continued)

439799-34-5 CAPLUS
1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 9-[[(2,4-dichlorophenyl)methoxy]imino]-1,2,3,4-tetrahydro-6-hydroxy-, 3-propyl
2-[2-(trimethylsilyl)ethyl] ester, (1R,2S,3S,4S,9E)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.

Relative stereochemistry.
Double bond geometry unknown

L12 ANSWER 1 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)
RN 439799-38-9 CAPLUS
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 1,2,3,4-tetrahydro-6,9dihydroxy-9-phenyl-, 3-propyl 2-[2-{trimethylsilyl}ethyl} ester,
(1R,2S,3S,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 439799-39-0 CAPLUS
CN 1.4-Ethanonaphthalene-2,3-dicarboxylic acid,
1.2.3,4-tetrahydro-6-hydroxy9-(propylamino)-, 3-propyl 2-[2-(trimethyleilyl)ethyl] ester,
(1R,2S,3S,4S,9R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 439799-42-5 CAPLUS
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid,
1,2,3,4-tetrahydro-6-hydroxy9-(phenylamino)-, 3-propyl 2-[2-(trimethylsilyl)ethyl] ester,
(1R,2S,3S,4S,9R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

433799-43-6 CAPLUS

1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 9-(dimethylamino)-1,2,3,4-tetrahydro-6-hydroxy-, 3-propyl 2-[2-(trimethylsilyl)ethyl] ester,
(1R,2S,3S,4S)-rel- (9CI) (CA INDEX NAME)

L12 ANSWER 1 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN

439799-49-2 CAPLUS
Spiro[1,3-dioxolane-2,2'(1'H)-[1,4]ethanonaphthalene]-9',10'-dicarboxylic
acid, 3',4'-dihydro-7'-hydroxy', 10'-propyl 9'-[2-(trimethylsilyl)ethyl]
ester, (1'R,4'S,9'R,10'R)-rel- (9CI) (CA INDEX NAME)

RN 439799-50-5 CAPLUS
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid,
9-(2-ethoxy-2-oxoethylidene)1,2,3,4-tetrahydro-6-hydroxy-, 3-propyl 2-[2-(trimethylsilyl)ethyl]

(1R, 2s, 3s, 4R) - rel - (9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry unknown

439799-51-6 CAPLUS

1,4-Ethanonaphthalene-2,3-dicarboxylic acid,
,3,4-tetrahydroo-6-hydroxy9-methylene-,3-propyl 2-[2-(trimethylsilyl)ethyl] ester,
(1R,2S,3S,4R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

L12 ANSWER 1 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

Relative stereochemistry.

439799-44-7 CAPLUS
1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 9-[acetyl](4-methylphenyl)methyl]amino]-6-(acetyloxy)-1,2,3,4-tetrahydro-, 3-propyl 2-[2-(trimethylsilyl)ethyl] eater, (1R,2S,3S,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 439799-46-9 CAPLUS
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid,
9-(acetylmethylamino)-1,2,3,4tetrahydro-6-hydroxy-,3-propyl 2-[2-(trimethylsilyl)ethyl] ester,
(1R,2S,3S,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

439/99-40-1 GARDS 1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 1,2,3,4-tetrahydro-6,9-dihydroxy-, 2:(2,4-dimethoxyphenyl)methyl) 2-(2-(trimethylsilyl)ethyl) ester, (IR,2S,3s,4s,8yR)-rel- (SCI) (CA INDEX NAME)

Relative stereochemistry.

L12 ANSWER 1 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 1,2,3,4-tetrahydro-6,9-dihydroxy-, 3-propyl 2-[2-(trimethylsilyl)ethyl) ester, (1R, 2S, 3S, 4S, 9R)-rel (9CI) (CA INDEX NAME)

Relative stereochemistry.

439799-53-8 CAPLUS (
1,4-Ethanonaphthalene-2;3-dicarboxylic acid,
ino-1,2,3,4-tetrahydro-6hydroxy-,3-propyl 2-(2-(trimethylsilyl)ethyl) ester, (1R,2S,3S,4S)-rel(9CI) (CA INDEX NAME)

Relative stereochemistry.

439799-54-9 CAPLUS 1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 1,2,3,4-tetrahydro-6,9-dihydroxy-9-methyl-, 3-propyl_2-[2-(trimethylaily1)ethyl] ester, (1R,2S,3S,4S,9R)-rel- (9CI) (CA INDEX NAME)

439799-56-1 CAPLUS
1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 1,2,3,4-tetrahydro-6,9-dihydroxy-9-methyl-, 3-propyl 2-[2-(trimethylsilyl)ethyl) ester, (1R,2S,3S,4S,9S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

439799-58-3 CAPLUS
1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 1,2,3,4-tetrahydro-6,9-dihydroxy-9-(hydroxymethyl)-, 3-propyl 2-(2-(trimethylsilyl)ethyl) ester, (lR,28,38,48,98)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

439799-59-4 CAPLUS
1,4-Ethanonaphthalene-2-carboxylic acid, 1,2,3,4-tetrahydro-7-hydroxy-3[methyl(phenylmethyl)amino]carbonyl}-10-oxo-, 2-propenyl ester,
[IR,ZR,3R,45]-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

L12 ANSWER 1 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

RN 439799-68-5 CAPLUS
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid,
1,2,3,4-tetrahydro-6-hydroxy9-oxo-, 3-propyl 2-{2-tricyclo[3.3.1.13,7]dec-1-ylethyl) ester,
(1R,2S,3S,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

439799-69-6 CAPLUS

1,4-Ethanonaphthalene-2,3-dicarboxylic acid,
3,4-tetrahydro-6-hydroxy9-oxo-,3-propyl 2-(3-(trimethylsilyl)propyl) ester, {1R,2S,3S,4S}-rel{9CI} (CA INDEX NAME)

Relative stereochemistry.

439799-71-0 CAPLUS
1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 6-{{4(carboxymethoxy)phenyl)methoxy}-1,2,3,4-tetrahydro-9-oxo-, 3-(2-propenyl)
2-{2-(trimethylsilyl)ethyl} ester, (1R,2S,3S,4S)-rel- (9CI) (CA INDEX

L12 ANSWER 1 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

439799-60-7 CAPLUS
1,4-Ethanonaphthalene-2-carboxylic acid, 1,2,3,4-tetrahydro-7-hydroxy-10-oxo-3-([propylamino]carbonyl]-, 2-propenyl ester, (1R,2R,3R,4S)-rel-

(9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 439799-64-1 CAPLUS
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid,
1,2,3,4-tetrahydro-6-hydroxy9-oxor, 2-[2-[4-methylphenyl)sulfonyl]ethyl] 3-propyl ester,
{1R,2S,3S,4S}-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 439799-66-3 CAPLUS
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid,
1,2,3,4-tetrahydro-6-hydroxy9-oxo-, 2-(3,3-dimethylbutyl) 3-propyl ester, (1R,2S,3S,4S)-rel- (9CI)
(CA INDEX NAME)

Relative stereochemistry

L12 ANSWER 1 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

Relative stereochemistry.

439799-75-4 CAPLUS
1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 6-(2-amino-2-oxoethoxy)1,2,3,4-tetrahydro-9-oxo-, 3-propyl 2-(2-(trimethylsilyl)ethyl) ester,
(lR,2S,3S,4S)-rel- (SCI) (CA INDEX NAME)

Relative stereochemistry.

439799-77-6 CAPLUS
1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 1,2,3,4-tetrahydro-6-(3-hydroxypropoxy)-9-oxo-, 3-propyl 2-[2-(trimethylsilyl)ethyl] ester, (IR,2S,3S,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

439799-82-3 CAPLUS
1,4-Ethanonaphthalene-2,3-dicarboxylic acid,
3,4-tetrahydro-6-hydroxy9-(propylamino)-, 3-propyl 2-[2-(trimethylsilyl)ethyl] ester,
(1R.2S,3S,4S,9S)-rel- (9CI) (CA INDEX NAME)

RN 439799-88-9 CAPLUS
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid,
1,2,3,4-tetrahydro-6-hydroxy9-(phenylaminol)-, 3-propyl 2-[2-(trimethylsilyl)ethyl] ester,
(1R,23,3S,4S,9S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 439799-91-4 CAPLUS
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 1,2,3,4-tetrahydro-6,9-dihydroxy-, 3-propyl 2-[2-(trimethylsilyl)ethyl] ester,
(1R,23,33,48,98)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 439800-16-5 CAPLUS
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid,
1,2,3,4-tetrahydro-6-hydroxy9-(methoxyimino)-, 3-propyl 2-[2-(trimethylsilyl)ethyl] ester,
{1R,2S,3S,4S,9Z}-rel-(9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.

L12 ANSWER 1 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

RN 439800-21-2 CAPLUS
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 1,2,3,4-tetrahydro-6,9-dihydroxy-, 2-[2-[(4-methylphenyl)sulfonyl]ethyl] 3-propyl ester, (1R,25,35,48)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 439800-22-3 CAPLUS
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid,
1,2,3,4-tetrahydro-6-hydroxy9-oxo-, 3-[(2,4-dimethoxyphenyl)methyl] 2-[2-(trimethylsilyl)ethyl]
ester,
(1R,2S,3R,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 439800-23-4 CAPLUS
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid,
1,2,3,4-tetrahydro-6-hydroxy9-oxo-, bis[2-(trimethylsilyl)ethyl) ester, (1R,2S,3R,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

L12 ANSWER 1 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

RN 439800-17-6 CAPLUS
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 9-[[(2,4-dichlorophenyl)]methoxylimino]-1,2,3,4-tetrahydro-6-hydroxy-, 3-propyl
2-[2-(trimethylsilyl)ethyl] ester, (1R,2S,3S,4S,92)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.

RN 439800-18-7 CAPLUS
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 1,2,3,4-tetrahydro-6,9-dihydroxy-, 3-[(2,4-dimethoxyphenyl)methyl] 2-[2-(trimethylsilyl)ethyl] ester, (1R,2S,3S,4S,9S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 439800-20-1 CAPLUS
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid,
9-(dimethylhydrazono)-1,2,3,4
tetrahydro-6-hydroxy-,2-[2-[{4-methylphenyl}sulfonyl]ethyl] 3-propyl
ester, (1R,2S,3S,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry unknown.

L12 ANSWER 1 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

RN 439800-24-5 CAPLUS
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid,
1,2,3,4-eterahydro-6-hydroxy9-oxo-, 3-(cyclopropylmethyl) 2-[2-(trimethylsilyl)ethyl] ester,
[IR,28,38,48)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 439800-26-7 CAPLUS
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid,
1,2,3,4-tetrahydro-6-hydroxy9-[(methoxycarbonyl)hydrazono]-, 3-propyl 2-{2-(trimethylsilyl)ethyl]
ester, (1R,2s,3s,4s)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry unknown.

RN 439800-27-8 CAPLUS
CN 1,4-Ethanonaphthalene-2,3-dicerboxylic acid,
1,2,3,4-tetrahydro-6-hydroxy9-[(2-oxo-2-(4-phenyl-1-piperazinyl)ethoxy]imino]-, 3-propyl
2-[2-(trimethyleilyl)ethyl] ester, (1R,25,35,45,92)-rel- (9CI) (CA INDEX NAME)

439800-28-9 CAPLUS
1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 1,2,3,4-tetrahydro-6,9-dihydroxy-9-(hydroxymethyl)-, 3-propyl 2-(2-(trimethylsilyl)ethyl) ester, (1R,2S,3S,4S,9S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

439919-18-3 CAPLUS
1,4-Ethanonaphthalene-2,3-dicarboxamide, 6-[[4-[[(2S)-2-

[{dimethylamino}carbonyl]-l-pyrrolidinyl]carbonyl]phenyl]methoxy]-1,2,3,4-tetrahydro-N2-methyl-9-oxo-N2-[2-oxo-2-[[(2,4,6-trimethoxyphenyl)methyl]amino]ethyl]-N3,N3-dipentyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L12 ANSWER 1 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

N-cyclohexylcyclohexanamine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 439798-61-5 CMF C19 H24 O6 Si

Relative stereochemistry.

CM 2

L12 ANSWER 1 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

PAGE 1-A

PAGE 1-B

439919-19-4 CAPLUS
1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 6-[[4-[[(2S)-2-

{ (dimethylamino) carbonyl}-1-pyrrolidinyl] carbonyl]phenyl]methoxy]-1,2,3,4-tetrahydro-9-oxo-, 3-propyl 2-(trimethylsilyl)ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L12 ANSWER 1 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

RN 439799-96-9 CAPLUS
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid,
1,2,3,4-tetrahydro-6-hydroxy9-oxo-, 2-{2-(trimethylsilyl)ethyl} ester, (1R,2S,3R,4S)-rel-, compd.

2-propanamine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 439798-61-5 CMF C19 H24 O6 Si

Relative stereochemistry.

NH2 нзс-сн-снз

439800-03-0 CAPLUS

1,4-Ethanonaphthalene-2,3-dicarboxylic acid,
(4-carboxyphenyl]methoxyl1,2,3,4-tetrahydro-9-oxo-, 3-propyl 2-[2-(trimethylsilyl)ethyl] ester,
(1R,2S,3S,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

439800-13-2 CAPLUS 1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 1,2,3,4-tetrahydro-6-[{4-{2-

L12 ANSWER 1 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

[2-[(4-methylphenyl)sulfonyl]ethoxy]-2-oxoethoxy]phenyl]methoxy]-9-o
3-(2-propenyl) 2-[2-(trimethylsilyl)ethyl] ester, (1R,2S,3S,4S)-rel-

(CA INDEX NAME)

Relative stereochemistry.

PAGE 1-A

PAGE 1-B

RN 439800-19-8 CAPLUS
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid,
1,2,3,4-tetrahydro-6-hydroxy9-[[(4-methylphenyl]methyl]amino]-, 3-propyl 2-[2-(trimethylsilyl)ethyl]
ester, (IR,2S,3S,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

L12 ANSWER 2 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN

AB A novel series of TMF-.alpha. inhibitors based on a benzobicyclooctane scaffold was reported. The compds. displayed good potency in inhibiting TMF-.alpha. induced apoptosis and Nf. kappa.B activation. Addnl., they were selective for TMF-.alpha. as they did not inhibit apoptosis induced by sol. Fas ligand. The compds. described here can act as leads for future medicinal chem. efforts and may also be useful tools for elucidating the TMF-.alpha. signaling pathway.

ACCESSION NUMBER: 2002:211239 CAPLUS

DOCUMENT NUMBER: 137:288467

TITLE: Benzobicyclooctanes as novel inhibitors of TMF-.alpha.

TITLE: TNF-.alpha.

signaling Jackson, Randy W.; Gelinas, Richard; Baughman, Ted AUTHOR(S):

Cox, Thomas; Howbert, J. Jeffry; Kucera, Kristin A.; Latham, John A.; Ramsdell, Fred; Singh, Devinder; Darwish, Ihab S. Department of Chemical Genomics, Celltech R&D, Inc., Bothell, WA, 98021, USA Bloorganic & Medicinal Chemistry Letters (2002), 12(7), 1093-1097 CODEN: BMCLES; ISSN: 0960-894X Elsevier Science Ltd. Journal English

CORPORATE SOURCE:

SOURCE:

PUBLISHER: DOCUMENT TYPE: LANGUAGE: IT 439798-62-

GUAGE: English
437798-62-6P
RI: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(att ohbenzobicyclooctanes as novel inhibitors of TNF-.alpha.
signaling)
437958-62-6 CAPJUS
1, 4-Ethanonaphthalene-2, 3-dicarboxylic acid,
3,4-tetrahydro-6-hydroxy9-0xo-, 3-[2-(trimethylsilyl)ethyl] ester, (1R,2S,3R,4S)-rel- (9CI) (CA
INDEX NAME)

Relative stereochemistry.

439798-72-8P 439798-75-IP 439798-78-4P
439799-66-3P 439799-69-6F 468086-81-9P
RL: PAC (Pharmacological activity), RCT (Reactant); SPN (Synthetic preparation); TRU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses) (benzobicyclooctanes as novel inhibitors of TNF-.alpha. signaling)
439798-72-8 CAPLUS
1,4-Ethanonaphthalene-2,3-dicarboxylic acid,
,3,4-ettrahydro-6-hydroxy9-oxo-,3-propyl 2-[2-(trimethylsilyl)ethyl] ester, (1R,2S,3S,4S)-rel(9CI) (CA INDEX NAME)

L12 ANSWER 1 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN RN 439800-29-0 CAPLUS (Continued)

RN 439800-29-0 CAPLUS
Cn 1.4-Ethanonaphthalene-2,3-dicarboxylic acid,
1,2,3,4-tetrahydro-6-hydroxy9-oxo-, 3-[2-(trimethylailyl)ethyl] ester, (1R,2S,3R,4S)-rel-, compd.

with N-cyclohexylcyclohexanamine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 439798-62-6 CMF C19 H24 O6 Si

Relative stereochemistry.

CM 2

CRN 101-83-7 CMF C12 H23 N

L12 ANSWER 2 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN (Continued) Relative stereochemistry.

RN 439798-75-1 CAPLUS
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid,
1,2,3,4-tetrahydro-6-hydroxy9-oxo-,3-[(3-fluorophenyl)methyl] 2-[2-(trimethylsilyl)ethyl] ester,
{1R,2S,3S,4S}-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

439798-78-4 CAPLUS
1,4-Ethanonaphthalene-2,3-dicarboxylic acid,
3,4-tetrahydro-6-hydroxy9-oxo-, 3-(2-propenyl) 2-[2-(trimethylsilyl)ethyl] ester,
(1R,2S,3S,4S)-rel-(9CI) (CA INDEX NAME)

Relative stereochemistry.

439799-66-3 CAPLUS
1,4-Ethanonaphthalene-2,3-dicarboxylic acid,
3,4-tetrahydro-6-hydroxy9-oxo-,2-(3,3-dimethylbutyl) 3-propyl ester, (1R,2S,3S,4S)-rel- (9CI)
(CA INDEX NAME)

L12 ANSWER 2 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN

RN 439799-69-6 CAPLUS
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid,
1,2,3,4-tetrahydro-6-hydroxy9-oxo-, 3-propyl 2-(3-(trimethylsilyl)propyl) ester, (1R,2S,3S,4S)-rel(9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 468086-81-9 CAPLUS
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid,
1,2,3,4-tetrahydro-6-hydroxy9-oxo-,3-[2-(4-morpholinyl]ethyl]2-[2-(trimethylsilyl)ethyl]ester,
(IR,ZS,35,45)-rel-(9CI) (CA INDEX NAME)

Relative stereochemistry.

364778-17-6P 439798-99-9P 439799-04-9P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU

L12 ANSWER 2 OF 16 CAPIUS COPYRIGHT 2003 ACS on STN (Continued A39799-08-3 CAPIUS (CONTINUED A19799-08-3 CAPIUS (CONTINUED A1979-08-6-12-pyrtidinylmethoxy)-, 3-propyl 2-[2-(trimethyl@ilyl)ethyl] ester, (1R, 2S, 3S, 4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

439798-61-5P 439798-79-5P 468086-79-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (benzobicyclooctanes as novel inhibitors of TNF-.alpha. signaling) 439798-61-5 CAPLUS
1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 7,3,4-tetrahydro-6-hydroxy-9-oxo-, 2-[2-(trimethylsily1)ethy1] ester, (1R,2S,3R,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

439798-79-5 CAPLUS
1,4-Ethanonaphthalene-2-carboxylic acid, 3-(azidocarbonyl)-1,2,3,4-tetrahydro-6-hydroxy-9-oxo-, 2-(trimethylsilyl)ethyl ester,
(1R,2S,3S,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

L12 ANSWER 2 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
(Uses)
(benzobicyclooctanes as novel inhibitors of TNF-.alpha. signaling)
RN 364778-17-6 CAPLUS
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 6-(carboxymethoxy)-1,2,3,4-tetrahydro-9-xov-, 3-propyl 2-[2-(trimethylsilyl)ethyl) ester,
(1R,2S,3S,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 439798-99-9 CAPLUS
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid,
1,2,3,4-tetrahydro-9-oxo-6-[2(2-pyridinyl)ethoxy|-,3-propyl 2-[2-(trimethylsilyl)ethyl] ester,
(1R,2S,3S,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 439799-04-9 CAPLUS
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid,
6-ethoxy-1,2,3,4-tetrahydro-9cxo-,3-propyl 2-[2-(trimethylsilyl)ethyl] ester, (1R,2S,3S,4S)-rel(9CI)

(CA INDEX NAME)

Relative stereochemistry.

L12 ANSWER 2 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

RN 468086-79-5 CAPLUS CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 1,2,3,4-tetrahydro-6-hydroxy-9-oxo-, 3-propyl ester, (1R,2S,3S,4S)-rel- (9CI) (CA INDEX NAME)

468086-80-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(benzobicyclooctanes as novel inhibitors of TNF-.alpha. signaling)
468086-80-9 CAPLUS
1,4-Ethanonaphthalene-2-carboxylic acid, 3-(aminocarbonyl)-1,2,3,4-tetrahydro-7-hydroxy-10-oxo-, propyl ester, (1R,2R,3R,4S)-rel- (9CI) (CA INDEX NAME)

REFERENCE COUNT:

THERE ARE 20 CITED REFERENCES AVAILABLE FOR

RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

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L12 ANSWER 3 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN

AB Several salt bridges obsd. in protein x-ray crystallog. structures showed a consistent pattern of a carboxylate, situated near the face of an arom ring, forming a bond to an arginine residue of a ligand. To det. the driving force for these complexes, 1H NMR or potentiometric binding titrms. were performed on solns. contg. N-acetyl arginine Me ester, N-acetyl lysine Me ester, guanidinium chloride, or KCl and one member of
                  series of diacidic templates, which had arom. or aliph. groups placed below their carboxylates. Only templates having an arom. ring were able to form a salt bridge in water. Although most of the obvious interactions, such as ionic and cation-pin, and ion desolvation are important factors, assocn. of an amino acid in water required the
                 ence
of the entire amino acid. This result suggests that the interaction
between the allph. portion of an amino acid and an arom. ring of a
template is an important component of complexation. Arom. templates also
transported N-acetyl arginine Me ester from water to 1-octanol. The
results of the transport studies are discussed in terms of potential
intermediate states that could lower some of the activation barriers of
protein folding.

2001-946675 Captus
protein fold
ACCESSION NUMBER:
DOCUMENT NUMBER:
TITLE:
                                                                                         2001:934675 CAPLUS
136:212473
                                                                                       136:212473
Carboxylates Stacked over Aromatic Rings Promote Salt Bridge Formation in Water
Thompson, Samuel E.: Smithrud, David B.
Department of Chemistry, University of Cincinnati, Cincinnati, OH, 45221-0172, USA
Journal of the American Chemical Society (2002), 124(3), 422-449
CODEN: JACSAT; ISSN: 0002-7863
American Chemical Society
Journal
English
 AUTHOR(S):
CORPORATE SOURCE:
 SOURCE:
  PUBLISHER:
 DOCUMENT TYPE:
LANGUAGE:
IT 402593-85-
                                                                                         English
  1: 40299J-85-SP
RL: BSU (Biological study, unclassified); PRP (Properties); SPN
(Synthetic
(Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(Interaction between aliph. amino acid and arom. ring of template play role in salt bridge formation in water)
RN 402593-65-5 CAPPUS
CN 9,10-Ethanoanthracene-11,12-dicarboxylic acid,
9,10-dihydroz,6-d-dhydroxy-
, (9R,10R,11S,12R)-rel- (9CI) (CA INDEX NAME)
 Relative stereochemistry.
 REFERENCE COUNT:
THIS
                                                                                          72
                                                                                                              THERE ARE 72 CITED REFERENCES AVAILABLE FOR
                                                                                                                RECORD. ALL CITATIONS AVAILABLE IN THE RE
  FORMAT
```

Relative stereochemistry.

IT 364778-17-6P

RE: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of carboxylic acids via a mild and selective method for the cleavage of tert-Bu esters)
364778-17-6 CAPLUS

RN 364778-17-6 CAPLUS
1,4-Ethanonaphthalene-2,3-dicarboxylic acid, 6-(carboxymethoxy)-1,2,3,4-tetrahydro-9-oxo-, 3-propyl 2-[2-(trimethylsilyl)ethyl] ester, (IR,2S,3S,4S)-rel- (SII) (CA INDEX NAME)

Relative stereochemistry.

L12 ANSWER 3 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

L12 ANSWER 4 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

REFERENCE COUNT:

THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

ANSWER 5 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN

A2,6-donor-acceptor-substituted anthracene, namely 6-methoxy-2anthracencearboxylate (I), was synthesized. The emission of this compd.
exhibits significant solvatochromism. The fluorescence band position and
intensity are also remarkably sensitive to H+. Irradn. of I in soln.
yields the syn and anti head-to-tail dimers exclusively. A synergistic
electronic effect between the donor and acceptor substituents is proposed
to operate on the photophys. and photochem. properties of I.

ACCESSION NUMBER:
1399: 428048 CAPLUS
DOCUMENT NUMBER:
131:184751
Synthesis, fluorescence properties, and head-to-tail
regioselectivity in the photodimerization of a
donor-acceptor-substituted anthracene
Inhels, Helko
CORPORATE SOURCE:
Institut Organische Chemie, Univ. Wurzburg, Wurzburg,
D-97074, Germany

Institut Organische Chemie, Univ. Wurzburg, Wurzbur D-97074, Germany European Journal of Organic Chemistry (1999), (7), 1595-1600 CODEN: EJOCFK; ISSN: 1434-193X Wiley-VCH Verlag GmbH Journal SOURCE:

PUBLISHER:

DOCUMENT TYPE: LANGUAGE:

DAGE: English
R SOURCE(S): CASREACT 131:184751
240121-93-1F 240121-94-2P OTHER SOURCE(S):

240121-93-1F 240121-94-2F
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn., fluorescence properties, and regioselective photodimerization of methoxyanthracenecarboxylate)
240121-93-1 CAPLUS

Relative stereochemistry.

240121-94-2 CAPLUS
9,10-Ethanoanthracene-2,11,12-tricarboxylic acid,
-dihvdro-6-methoxy-, dihydro-6-methoxy-, (11R,12R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

REFERENCE COUNT: THIS

61 THERE ARE 61 CITED REFERENCES AVAILABLE FOR

L12 ANSWER 6 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN GI

The cycloaddn. of fumarates I (R1, R2 = cis-cyclohexylcylhexyl or trans-cyclohexylcyclohexyl, cholesteryl, etc.) with 2,6-dialkoxyanthracenes gave the syn-adducts II (same R1, R2; R3 = alkyl) and the corresponding anti-adducts. The ability of liq. cryst. solvent

the corresponding anti-adducts. The ability of liq. cryst. Solvent es to control the stereochem. course of bimol. thermal reactions of 2,6-dialkoxyanthracenes with a series of fumarates conducted at 130-180 .degree.C was examd., primarily with respect to the structural compatibility of the solutes with the solvent mesogens. For the case of the model thermal [4+2] cycloaddns. of 2,6-bis(decyloxy)anthracene to bis(trans-4-cyclohexylcyclohexyl) and cholesteryl trans-4-cyclohexylcyclohexyl fumarates at 130-150 .degree.C, cholesteryl 2,4-dichlorobenzoate (CDCB) and bis(4-pentylloxyphenyl) trans-1,4-cyclohexanedicarboxylate (BPCD) serve well as cholesteric and smectic liq. cryst. solvents and result in the preferential formation of syn-isomers with an extremely high level of regioselection (syn/anti.gtoreq. 20/1). In contrast, the isotropic solvents with closely related structures gave isomer ratios of only gloreq.3/1. Structural similarities between the solutes and the solvent mesogens appeared to

play

a key and influential role in controlling the stereochem. course of the
reaction. The temp. dependence for the isomer distribution afforded an
est. of the differences of solvation enthalpy and entropy between syn and
anti transition states in the anisotropic media.

ACCESSION NUMBER: 1996:311607 CAPLUS

DOCUMENT NUMBER: 125:57663

Liquid Crustal Control of Birelevilar Mineral

Liquid Crustal Control of Birelevilar Mineral

DOCUMENT NUMBER: TITLE:

125:57663
Liquid Crystal Control of Bimolecular Thermal
Reactions. Highly Regioselective Pericycloaddition of
Fumarates to 2,6-Dialkoxyanthracenes in
Liquid-Crystalline Media
Kansui, Hisao: Hiraoka, Shingo: Kunieda, Takehisa
Faculty of Pharmaceutical Sciences, Kumamoto
University, Kumamoto, 862, Japan
Journal of the American Chemical Society (1996),
118(23), 5346-5352
CODEN: JACSAT; ISSN: 0002-7863
American Chemical Society
Journal

AUTHOR(S): CORPORATE SOURCE:

PUBLISHER:

DOCUMENT TYPE: LANGUAGE: English 143878-98-2P 143878-99-3P 143879-00-9P 143879-01-0P 143955-32-2P 143955-33-3P

play

SOURCE:

L12 ANSWER 5 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN (Continued) RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 6 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)
143955-34-4P 143955-35-5P 178099-93-9P
178099-94-0P 178099-98-4P 178099-98-5P
178099-97-3P 178099-98-4P 178099-99-5P
178230-35-8P 178230-35-9P 178230-37-0P
178230-38-1P 178230-39-2P 178230-40-5P
178230-41-6P 178230-42-7P 178230-43-8P
178230-44-9P 178230-45-0P 178230-46-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(thermal pericycloaddn. of fumarates to dialkoxyanthracenes in presence (thermal pericycloaddn. of fumarates to dia presence
of liq. crystal solvents)
RN 143878-98-2 CAPFUS
CN 9,10-Ethanoanthracene-11,12-dicarboxylic acid,
2,6-dibutoxy-9,10-dihydro-,
bis([1,1'-bicyclohexyl]-4-yl) ester,
[9.alpha.,10.alpha.,115' (trans), 125' (
trans)]- (9CI) (CA INDEX NAME)

Relative stereochemistry

143878-99-3 CAPLUS 9,10-Ethanoanthracene-11,12-dicarboxylic acid, 2,6-bis(decyloxy)-9,10-dihydro-, bis([1,1'-bicyclohexyl]-4-yl) ester, [9.alpha.,10.alpha.,118*(trans),128*(trans)]- (9CI) (CA INDEX NAME)

Relative stereochemistry.

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

PAGE 2-A

RN 143879-00-9 CAPLUS
CN 9,10-Ethanoanthracene-11,12-dicarboxylic acid,
2,6-dibutoxy-9,10-dihydro-,
{1,1*-bicyclohexyl}-4-yl 4-methoxyphenyl ester,
{9.alpha.,10.alpha.,11S*(trans),123*]- (9CI) (CA INDEX NAME)

Relative stereochemistry.

143879-01-0 CAPLUS
9,10-Ethanoanthracene-11,12-dicarboxylic acid, 2,6-bis(decyloxy)-9,10-dihydro-, [1,1'-bicyclohexyl]-4-yl 4-methoxyphenyl ester,
[9,alpha.,10.alpha.,115*(trans),125*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

L12 ANSWER 6 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

RN 143955-34-4 CAPLUS
CN 9,10-Ethanoanthracene-11,12-dicarboxylic acid,
2,6-dibutoxy-9,10-dihydro-,
[1,1'-bicyclohexyl]-4-yl 4-methoxyphenyl ester,
[9.alpha.,10.alpha.,11R*(trans),12R*]- (9CI) (CA INDEX NAME)

143955-35-5 CAPLUS
9,10-Ethanoanthracene-11,12-dicarboxylic acid, 2,6-bis(decyloxy)-9,10-dihydro-, [1,1'-bicyclohexyl]-4-yl 4-methoxyphenyl ester,
[9.alpha.,10.alpha.,11R*(trans),12R*]- (9CI) (CA INDEX NAME)

Relative stereochemistry.

L12 ANSWER 6 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

RN 143955-32-2 CAPLUS
CN 9,10-Ethanoanthracene-11,12-dicarboxylic acid,
2,6-dibutoxy-9,10-dihydro-,
bis([1,1'-bicyclohexyl]-4-yl) ester,
[9.alpha.,10.alpha.,118*(trans),12R*(
trans)]- (9CI) (CA INDEX NAME)

143955-33-3 CAPLUS
9,10-Ethanoanthracene-11,12-dicarboxylic acid, 2,6-bis(decyloxy)-9,10-dihydro-, bis([1,1'-bicyclohexyl]-4-yl) ester,
[9.alpha.,10.alpha.,11R*(trans),12R*(trans)]- (9CI) (CA INDEX NAME)

L12 ANSWER 6 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

PAGE 1-A

PAGE 1-B

PAGE 1-C

178099-93-9 CAPLUS
9,10-Ethanoanthracene-11,12-dicarboxylic acid, 9,10-dihydro-2,6-bis(2-methoxyethoxy)-, bis[1,1'-bicyclohexyl]-4-yl ester,
[9,alpha.,10.alpha.,115*(trans),125*(trans))- (9CI) (CA INDEX NAME)

Relative stereochemistry.

178099-94-0 CAPLUS (Cholest-5-en-3-ol (3.beta.)-, 12-[1,1'-biphenyl]-4-yl 3,7-bis(decyloxy)-9,10-dhydro-9,10-ethanoanthracene-11,12-dicarboxylate (9CI) (CA INDEX

Absolute stereochemistry.

L12 ANSWER 6 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN

178099-96-2 CAPLUS
9,10-Ethanoanthracene-11,12-dicarboxylic acid, 2,6-bis(decyloxy)-9,10-dihydro-, dicyclohexyl ester, (9.alpha.,10.alpha.,115*,125*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

178099-97-3 CAPLUS
9,10-Ethanoanthracene-11,12-dicarboxylic acid, 2,6-bis(decyloxy)-9,10-dihydro-, dioctyl ester, (9.alpha.,10.alpha.,115*,125*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

L12 ANSWER 6 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

PAGE 1-A

PAGE 1-B

178099-95-1 CAPLUS
9,10-Ethanoanthracene-11,12-dicarboxylic acid, 2,6-bis(decyloxy)-9,10-dihydro-, [1,1*-bicyclohexyl]-4-yl [1,1*-biphenyl]-4-yl ester, [9.alpha.,10.alpha.,115*(trans),125*]- (9CI) (CA INDEX NAME)

Relative stereochemistry.

L12 ANSWER 6 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)
RN 178099-98-4 CAPLUS
CN 9,10-Ethanoanthracene-11,12-dicarboxylic acid, 2,6-bis(decyloxy)-9,10-dihydro-, bis(1-pentylhexyl) ester, (9.alpha.,10.alpha.,11S*,12S*)- (9CI)
(CA INDEX NAME)

178099-99-5 CAPLUS 9,10-Ethanoanthracene-11,12-dicarboxylic acid, 2,6-bis(decyloxy)-9,10-dihydro-, [1,1'-bicyclohexyl]-4-yl 3-cyclohexylpropyl ester, [9.alpha.,10.alpha.,115'(trans),125')- (9CI) (CA INDEX NAME)

Relative stereochemistry.

178230-35-8 CAPLUS
Cholest-5-en-3-ol (3.beta.)-, [1,1'-bicyclohexyl]-4-yl
2,6-bis(decyloxy)-9,10-dihydro-9,10-ethanoanthracene-11,12-dicarboxylate
(SCI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

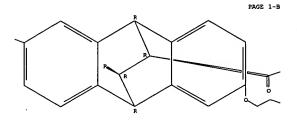
PAGE 1-B

-(CH₂)3 CHMe₂

178230-36-9 CAPLUS
Cholest-5-en-3-ol (3.beta.)-, [1,1'-bicyclohexyl]-4-yl
2,6-dibutoxy-9,10-dihydro-9,10-ethanoanthracene-11,12-dicarboxylate (9CI)
(CA INDEX NAME)

Absolute stereochemistry.

L12 ANSWER 6 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



PAGE 1-C

PAGE 2-A

178230-38-1 CAPLUS
9,10-Ethanoanthracene-11,12-dicarboxylic acid, 2,6-bis(decyloxy)-9,10-dihydro-, bis([1,1'-blcyclohexyl]-4-yl) ester,
[9.alpha.,10.alpha.,115*(cis),125*(cis)]- (9CI) (CA INDEX NAME)

Relative stereochemistry.

L12 ANSWER 6 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

PAGE 1-A

PAGE 1-B

- (CH2) 3 CHMe2

178230-37-0 CAPLUS
9,10-Ethanoanthracene-11,12-dicarboxylic acid, 9,10-dihydro-2,6-bis(2-methoxyethoxy)-, bis(1,1'-bicyclohexyl)-4-yl) ester,
[9.alpha.,10.alpha.,11R*(trans),12R*(trans)]- (9CI) (CA INDEX NAME)

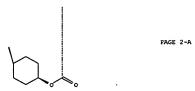
Relative stereochemistry.

PAGE 1-A



L12 ANSWER 6 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *



178230-39-2 CAPLUS
9,10-Ethanoanthracene-11,12-dicarboxylic acid, 2,6-bis(decyloxy)-9,10-dihydro-,bis([1,1'-bicyclohexyl]-4-yl) ester,
[9.alpha.,10.alpha.,11R*(cis),12R*(cis)]- (9CI) (CA INDEX NAME)

178230-40-5 CAPLUS
9,10-Ethanoanthracene-11,12-dicarboxylic acid, 2,6-bis(decyloxy)-9,10-dihydro-, (1,1'-bicyclohexyl)-4-yl [1,1'-biphenyl]-4-yl ester, [9.alpha.,10.alpha.,11R*(trans),12R*]- (9CI) (CA INDEX NAME)

L12 ANSWER 6 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN

(Continued) PAGE 1-A

(CH₂) 9 0

PAGE 1-C

L12 ANSWER 6 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

PAGE 1-A

PAGE 1-B

∼cHMe2

178230-43-8 CAPLUS
9,10-Ethanoanthracene-11,12-dicarboxylic acid, 2,6-bia(decyloxy)-9,10-dihydro-, dlcyclohexyl ester, (9.alpha.,10.alpha.,11R*,12R*)- (9CI) (CA INDEX NAME)

L12 ANSWER 6 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

PAGE 2-A

178230-41-6 CAPLUS
Cholest-5-en-3-ol (3.beta.)-, 4-methoxyphenyl 2,6-bis(decyloxy)-9,10-dihydro-9,10-ethanoanthracene-11,12-dicarboxylate (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 1-B

RN 178230-42-7 CAPLUS Cholest-9, 4-methoxyphenyl 2,6-dibutoxy-9,10-dihydro-9,10-ethanoanthracene-11,12-dicarboxylate (9C1) (CA INDEX NAME)

L12 ANSWER 6 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

178230-44-9 CAPLUS
9,10-Ethanoanthracene-11,12-dicarboxylic acid, 2,6-bis(decyloxy)-9,10-dihydro-, dioctyl ester, (9.alpha.,10.alpha.,11R*,12R*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

178230-45-0 CAPLUS
9.10-Ethanoanthracene-11,12-dicarboxylic acid, 2,6-bis(decyloxy)-9,10-dihydro-, bis(1-pentylhexyl) ester, (9.alpha.,10.alpha.,11R*,12R*)- (9CI) (CA INDEX NAME)

178230-46-1 CAPLUS
9,10-Ethanoanthracene-11,12-dicarboxylic acid, 2,6-bis(decyloxy)-9,10-dihydro-, (1,1'-bicyclohexyl)-4-yl 3-cyclohexylpropyl ester, (9,alpha.,11R*(trans),12R*)- (9CI) (CA INDEX NAME)

L12 ANSWER 7 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

CM 2

C1-C-(CH₂)8-C-C1

176391-77-8 CAPLUS

CN
Poly[oxy[9,10-bis(acetyloxy)-9,10-dihydro-11,12-bis(methoxycarbonyl)-9,10ethanoanthracene-2,6-diyl]oxy(1,10-dioxo-1,10-decanediyl)] (9CI) (CA
INDEX NAME)

RN 176391-78-9 CAPLUS
CN 9,10-Ethanoanthracene-11,12-dicarboxylic acid, 9,10-bis(acetyloxy)-9,10-dihydro-2,6-dihydroxy-, dimethyl ester, polymer with 1,4-benzenedicarbonyl dichloride (9CI) (CA INDEX NAME)

CM 1

CRN 176391-74-5

L12 ANSWER 7 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN

AB Sol. polyesters are synthesized by polymg, a range of bis(acid chloride)s with the bisphenol that is formally the Diels-Alder adduct of 9,10-diacetoxy-2,6-dihydroxyanthracene and dl-Me maleate. Heating the sol. polyesters to about 230.degree. brought about retro-Diels-Alder reactions to give the insol. target polyesters contg. 9,10-diacetoxyanthracene residues.

ACCESSION NUMBER: 1996:257386 CAPLUS
DOCUMENT NUMBER: 124:318058 24:318058

Synthesis of polyesters containing
9,10-diacetoxyanthracene-2,6-diyl moieties via a
precursor polymer approach
Uddin, Rush; Hodge, Phillip; Chisholm, Michael S.;
Eustace, Paul
Chem. Dep., Univ. Manchester, Manchester, M12 9PL, UK
JOurnal of Materials Chemistry (1996), 6(4), 527-32
CODEN: JMACEF, ISSN: 0959-9428
Royal Society of Chemistry
Journal English AUTHOR (S):

CORPORATE SOURCE: SOURCE:

PUBLISHER: DOCUMENT TYPE: LANGUAGE: IT 176391-74-5P English

176391-74-59
RE: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(monomer; synthesis of polyesters contg. 9,10-diacetoxyanthracene-2,6-diyl moieties via precursor and retro-Diela-Alder reaction)
176391-74-5 CAPLUS
9,10-Ethanoanthracene-11,12-dicarboxylic acid, 9,10-bis(acetyloxy)-9,10-dihydro-2,6-dihydroxy-, dimethyl ester (9CI) (CA INDEX NAME)

CM 1

L12 ANSWER 7 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN CMF C24 H22 010 (Continued)

CM 2

CRN 100-20-9 CMF C8 H4 C12 O2

RN 176391-79-0 CAPLUS
CN
Poly[oxycarbonyl-1, 4-phenylenecarbonyloxy[9,10-bis(acetyloxy)-9,10-dihydro11,12-bis(methoxycarbonyl)-9,10-ethanoanthracene-2,6-diyl]] (9CI) (CA

176391-80-3 CAPLUS

NN 176391-80-3 CAPLOS ON 9,10-Ethanoanthracene-11,12-dicarboxylic acid, 9,10-bis(acetyloxy)-9,10-dihydro-2,6-dihydroxy-, dimethyl ester, polymer with dichloride (9CI) (CA INDEX NAME)

CH 1

CRN 176391-74-5 CMF C24 H22 O10

CM 2

CRN 99-63-8 CMF C8 H4 C12 O2

RN 176391-81-4 CAPLUS
CN
Poly[oxycarbonyl-1,3-phenylenecarbonyloxy[9,10-bis(acetyloxy)-9,10-dihydro11,12-bis(methoxycarbonyl)-9,10-ethanoanthracene-2,6-diyl]] (9CI) (CA
INDEX NAME)

RN 176391-82-5 CAPLUS
CN 9,10-Ethanoanthracene-11,12-dicarboxylic acid, 9,10-bis(acetyloxy)-9,10-dihydroz,6-dihydroxy-, dimethyl ester, polymer with 1,2-benzenedicarbonyl

L12 ANSWER 7 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)
RN 176391-84-7 CAPLUS
CN 9,10-Ethanoanthracene-11,12-dicarboxylic acid, 9,10-bis(acetyloxy)-9,10dihydro-2,6-dihydroxy-, dimethyl ester, polymer with hexanedicyl
dichloride (9CI) (CA INDEX NAME)

CM 1

CRN 176391-74-5 CMF C24 H22 010

CM 2

CRN 111-50-2 CMF C6 H8 C12 O2

176391-85-8 CAPLUS
Poly[oxy(1,6-dioxo-1,6-hexanediy1]oxy[9,10-bis(acetyloxy)-9,10-dihydro11,12-bis(methoxycarbony1)-9,10-ethanoanthracene-2,6-diy1]] (9CI) (CA
INDEX NAME)

RN 176391-86-9 CAPLUS
CN 9,10-Ethanoanthracene-11,12-dicarboxylic acid, 9,10-bis(acetyloxy)-9,10-dihydro-2,6-dihydroxy-, dimethyl ester, polymer with
[1,1'-bipheny1]-4,4'-

L12 ANSWER 7 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN dichloride (9CI) (CA INDEX NAME) (Continued)

CM 1

CRN 176391-74-5 CMF C24 H22 O10

CM 2

CRN 88-95-9 CMF C8 H4 C12 O2

RN 176391-83-6 CAPLUS
CN
Poly[oxycarbonyl-1,2-phenylenecarbonyloxy[9,10-bis(acetyloxy)-9,10-dihydro11,12-bis(methoxycarbonyl)-9,10-ethanoanthracene-2,6-diyl]} (9CI) (CA
INDEX NAME)

L12 ANSWER 7 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN dicarbonyl dichloride (9CI) (CA INDEX NAME) (Continued)

CM 1

CRN 176391-74-5 CMF C24 H22 O10

CM 2

CRN 2351-37-3 CMF C14 H8 C12 O2

RN 176391-87-0 CAPLUS
CN
Poly[oxy[9,10-bis(acetyloxy)-9,10-dihydro-11,12-bis(methoxycarbonyl)-9,10-ethanoanthracene-2,6-diyl]oxycarbonyl[1,1'-biphenyl]-4,4'-diylcarbonyl]
(9CI) (CA INDEX NAME)

176391-88-1 CAPLUS
9,10-Ethanoanthracene-11,12-dicarboxylic acid, 9,10-bis(acetyloxy)-9,10-dihydro-2,6-dihydroxy-, dimethyl ester, polymer with 4,4'-oxybis[benzoyl

L12 ANSWER 7 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN chloride) (9CI) (CA INDEX NAME) (Continued)

CM 1

CRN 176391-74-5 CMF C24 H22 O10

CM 2

CRN 7158-32-9 CMF C14 H8 C12 03

176391-89-2 CAPLUS
Poly(oxycarbonyl-1, 4-phenyleneoxy-1, 4-phenylenecarbonyloxy[9, 10-bis(acetyloxy)-9, 10-dihydro-11, 12-bis(methoxycarbonyl)-9, 10-ethanoanthracene-2, 6-diyl]] (9CI) (CA INDEX NAME)

176391-90-5 CAPLUS

176391-90-5 CAPIUS
9,10-Ethanoanthracene-11,12-dicarboxylic acid, 9,10-bis(acetyloxy)-9,10-dihydro-2,6-dihydroxy-, dimethyl ester, polymer with 2,6-naphthalenedicarbonyl dichloride (9CI) (CA INDEX NAME)

ANSWER 7 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(prepn. and esterification of)
176391-75-6 CAPLUS
9,10-Ethanoanthracene-11,12-dicarboxylic acid, 9,10-bis(acetyloxy)-9,10-dihydro-2,6-dihydroxy-, monomethyl ester (9CI) (CA INDEX NAME)

CM 1

CRN 176391-74-5 CMF C24 H22 O10

L12 ANSWER 7 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

CM 1

CRN 176391-74-5 CMF C24 H22 O10

CM 2

RN 176391-91-6 CAPLUS
CN.
Poly[oxy[9,10-bis(acetyloxy)-9,10-dihydro-11,12-bis(methoxycarbonyl)-9,10-ethanoanthracene-2,6-diyl]oxycarbonyl-2,6-naphthalenediylcarbonyl] (9CI)
(CA INDEX NAME)

IT 176391-75-6P

L12 ANSWER 7 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

CM 2

CRN 111-19-3 CMF C10 H16 C12 O2

176391-77-8 CAPLUS

Poly[oxy[9,10-bis(acetyloxy)-9,10-dihydro-11,12-bis(methoxycarbonyl)-9,10-ethanoanthracene-2,6-diyl]oxy(1,10-dioxo-1,10-decanediyl)] (9CI) (CA INDEX NAME)

RN 176391-78-9 CAPLUS
CN 9,10-Ethanoanthracene-11,12-dicarboxylic acid, 9,10-bis(acetyloxy)-9,10-dihydro-2,6-dihydroxy-, dimethyl ester, polymer with 1,4-benzenedicarbonyl dichloride (9CI) (CA INDEX NAME)

CM 1

CRN 176391-74-5 CMF C24 H22 O10

CM 2

176391-79-0 CAPLUS

RN 176391-79-0 CAPLUS
CN
Poly[oxycarbonyl-1,4-phenylenecarbonyloxy[9,10-bis(acetyloxy)-9,10-dihydro11,12-bis(methoxycarbonyl)-9,10-ethanoanthracene-2,6-diyl]] (9CI) (CA
INDEX NAME)
•

RN, 176391-80-3 CAPLUS
ON 9,10-Ethanoanthracene-11,12-dicarboxylic acid, 9,10-bis(acetyloxy)-9,10-dixydro-2,6-dihydroxy-, dimethyl ester, polymer with
1,3-benzenedicarboxyl
dichloride (9C1) (CA INDEX NAME)

CM 1

CRN 176391-74-5 CMF C24 H22 O10

L12 ANSWER 7 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

CM 2

CRN 88-95-9 CMF C8 H4 C12 O2

RN 176391-83-6 CAPLUS
CN
Poly(oxycarbonyl-1,2-phenylenecarbonyloxy[9,10-bis(acetyloxy)-9,10-dihydro11,12-bis(methoxycarbonyl)-9,10-ethanoanthracene-2,6-diyl]] (9CI) (CA
INDEX NAME)

176391-84-7 CAPLUS 9,10-Ethanoanthracene-11,12-dicarboxylic acid, 9,10-bis(acetyloxy)-9,10-dihydro-2,6-dihydroxy-, dimethyl ester, polymer with hexanedioyl dichloride (9CI) (CA INDEX NAME)

CM 1

L12 ANSWER 7 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

2

CRN 99-63-8 CMF C8 H4 C12 O2

RN 176391-81-4 CAPLUS
CN
Poly[oxycarbonyl-1,3-phenylenecarbonyloxy[9,10-bis[acetyloxy]-9,10-dihydro11,12-bis[methoxycarbonyl)-9,10-ethanoanthracene-2,6-diyl]] [9CI] (CA
INDEX NAME)

RN 176391-82-5 CAPLUS
CN 9,10-Ethanoanthracene-11,12-dicarboxylic acid, 9,10-bis(acetyloxy)-9,10-dihydro-2,6-dihydroxy-, dimethyl ester, polymer with
1,2-benzenedicarbonyl
dichloride (9CI) (CA INDEX NAME)

CM 1

CRN 176391-74-5 CMF C24 H22 O10

L12 ANSWER 7 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

CRN 176391-74-5 CMF C24 H22 O10

CM 2

CRN 111-50-2 CMF C6 H8 C12 O2

176391-85-8 CAPLUS
Poly[oxy(1,6-dioxo-1,6-hexanediy1]oxy[9,10-bis(acetyloxy)-9,10-dihydro-11,12-bis(methoxycarbony1)-9,10-ethanoanthracene-2,6-diy1]] (9CI) (CA INDEX NAME)

RN 176391-86-9 CAPLUS
9,10-Ethanoanthracene-11,12-dicarboxylic acid, 9,10-bis(acetyloxy)-9,10-dihydro-2,6-dihydroxy-, dimethyl ester, polymer with
{1,1'-biphenyl|-4,4'dicarbonyl dichloride (9CI) (CA INDEX NAME)

CM 1

CRN 176391-74-5 CMF C24 H22 O10

CM 2

CRN 2351-37-3 CMF C14 H8 C12 O2

RN 176391-87-0 CAPLUS CN Poly[oxy] 9, 10-dihydro-11, 12-bis(methoxycarbonyl) -9, 10-ethanoanthracene-2, 6-diyl] oxycarbonyl[1, 1*-biphenyl] -4, 4*-diylcarbonyl] (9CI) (CA INDEX NAME)

176391-88-1 CAPLUS 9,10-Ethanoanthracene-11,12-dicarboxylic acid, 9,10-bis(acetyloxy)-9,10-dihydro-2,6-dihydroxy-, dimethyl ester, polymer with 4,4'-oxybis[benzoyl chloride] (9C1) (CA INDEX NAME)

CM 1

CRN 176391-74-5 CMF C24 H22 O10

L12 ANSWER 7 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

CN 2

CRN 2351-36-2 CMF C12 H6 C12 O2

RN 176391-91-6 CAPLUS
CN
Poly{oxy[9,10-bis(acetyloxy)-9,10-dihydro-11,12-bis(methoxycarbonyl)-9,10-ethanoanthracene-2,6-diyl]oxycarbonyl-2,6-naphthalenediylcarbonyl] (9CI)
(CA INDEX NAME)

CRN 7158-32-9 CMF C14 H8 C12 O3

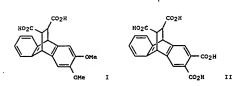
176391-89-2 CAPLUS
Poly(oxycarbonyl-1, 4-phenyleneoxy-1, 4-phenylenecarbonyloxy[9, 10-bis(acetyloxy)-9, 10-dihydro-11, 12-bis(methoxycarbonyl)-9, 10-ethanoanthracene-2, 6-diyl]] (9CI) (CA INDEX NAME)

176391-90-5 CAPLUS 9,10-Ethanoanthracene-11,12-dicarboxylic acid, 9,10-bis(acetyloxy)-9,10-dihydro-2,6-dihydroxy-, dimethyl ester, polymer with 2,6-naphthalenedicarbonyl dichloride (9CI) (CA INDEX NAME)

CM 1

CRN 176391-74-5 CMF C24 H22 O10

L12 ANSWER 8 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN



AD efficient oxidm. of Me and primary side chains of anthracene
Diels-Alder adducts with NothO4 is reported (e.g., I .fwdarw. II). The
oxidm. leaves the bridgehead methine intact providing Diels-Alder adducts
of anthracenecarboxylic acids. Retro Diels-Alder reaction allows for the
preps. of the parent anthracenecarboxylic acids.

ACCESSION NUMBER: 1994:700572 CAPLUS
DOCUMENT NUMBER: 121:300572
Oxidation of aliphatic side chains in anthracene
Diels-Alder adducts
AUTHOR(S): McCommick, Frankie A.: Marquardt, Donald J.
CORPORATE SOURCE: Dep. Chem., Tulane Univ., New Orleans, LA, 70118, USA
SOURCE: CODEN: TELERY; ISSN: 0040-4039
DOCUMENT TIPE: Journal

CODEN: TELEARY ISSN: 0040-4039

DOCUMENT TYPE:
JOURNAL
JOURNAL
LANGUAGE:
English
OTHER SOURCE(S): English
OTHER SOURCE(S): CASREACT 121:300572

RL: RCT (Reactant): RACT (Reactant or reagent)
(regioselective oxidn. of aliph. side chains in anthracene Diels-Alder
adducts with potassium permanganate)
RN 159046-93-4 CAPLUS
CN 9,10-Ethanoanthracene-11,12-dicarboxylic acid,
9,10-dihydro-4,6-dimethoxy1,2-dimethyl-, (9.alpha.,10.alpha.,118*,125*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

(Continued)

L12 ANSWER B OF 16 CAPLUS COPYRIGHT 2003 ACS on STN

159169-20-7 CAPLUS

RN 159169-20-7 CAPLUS
C1 9,10-Ethanoanthracene-11,12-dicarboxylic acid,
9,10-dihydro-4,6-dimethoxy1,2-dimethyl-, (9.alpha.,10.alpha.,11R*,12R*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

139047-05-9P 159169-25-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(regioselective oxidn. of aliph. side chains in anthracene Diela-Alder adducts with potassium permanganate)
159047-05-9 CAPIUS
9,10-Ethanoanthracene-1,2,11,12-tetracarboxylic acid, 9,10-dihydro-4,6-dimethoxy-, (9.alpha.,10.alpha.,115*,125*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

159169-25-2 CAPLUS
9,10-Ethanoanthracene-1,2,11,12-tetracarboxylic acid, 9,10-dihydro-4,6-dimethoxy-, (9.alpha.,10.alpha.,11R*,12R*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

ANSWER 9 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN

The authors describe a large no. of binding studies in aq. media designed to provide new insights into noncovalent binding interactions, esp. the cation-pi. interaction. The studies include 7 different hosts, >70 guests, and >150 new binding consts. In addn. to the now std. NMR methods, CD was an esp. useful tool for detg. aq. binding consts. In addn. to the alkyliminium and tetraalkylammonium guests studied previously, sulfonium and quantidnium guests also show substantial cation-pi. effects. Bromination of the host greatly enhances its binding

binding ability in a general fashion, primarily as a result of hydrophobic interactions. Addn. of methoxy groups did not enhance binding,

ability in a general results, presents, presents, addn. of methoxy groups did not enhance binding, apparently as a result of a collapse of the host into a conformation that is not suitable for binding. Replacement of two benzene rings of the host by furans or thiophenes also did not enhance binding. Ab initio calcus, provide a rationalization for this effect and suggest a clearer model for the cation-pi. interaction.

ACCESSION NUMBER: 1994/8143 CAPLUS
DOCUMENT NUMBER: 120:8143
Molecular recognition in aqueous media. New binding studies provide further insights into the cation-pi. interaction and related phenomena A.; Forman, Jonathan E.; McCurdy, Alison; Dougherty, Dennis A.

CORPORATE SOURCE: Arnold Mabel Beckman Lab. Chem. Synth., California Inst. Technol., Pasadena, CA, 91125, USA
Journal of the American Chemical Society (1993), 115(22), 9907-19
CORDENT TYPE: JOURNAL SPACE AND SP

UNGE: Journal
UNGE: English
151424-30-5F 151529-74-7F
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(prepn. and oxidn. of)
151424-30-5 CAPLUS
9.10-Ethanoanthreament)

RN 151424-30-5 CAPLUS
On 9,10-Ethanoanthracene-11,12-dicarboxylic acid, 1,5-dibromo-2,6-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]-9,10-dihydro-, bis[5-methyl-2-(1-methylethyl)cyclohexy] ester,
[9R-[9.alpha,10.alpha,11s*(18*,25*,5R*),1
23*(1R*,25*,5R*)]]- (9CI) (CA INDEX NAME)

L12 ANSWER 9 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

RN 151529-74-7 CAPLUS
CN 9,10-Ethanoanthracene-11,12-dicarboxylic acid, 1,5-dibromo-2,6-bis[{{1,1-dimethylethyl|dimethyleilyl|oxy}-9,10-dihydro-, bis[5-methyl-2-{1-methylethyl|cyclohexyl] ester,
[9s-[9.alpha.,10.alpha.,115-{118-{25-58-1,1}
25*(1R*,25*,5R*)]]- (9CI) (CA INDEX NAME)

ANSWER 10 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN
AB Mol. ordering present in cholesteric liq. cryst. solvent phase is shown to AB Mol. ordering present in cholesteric liq. cryst. solvent phase is shown to be rigid enough to regulate the uncatalyzed Diels-Alder reactions of cholesteryl and 4-cyclohexylcyclohexyl fumarates with 2,6-dialkoxyanthracenes conducted above 130.degree. with significantly high regioselectivity up to 90% d.e., which is considerably dependent on the structural features of reactants and the mesogens.

ACCESSION NUMBER: 1992:591441 CAPLUS

DOCUMENT NUMBER: 117:191441

Strong regiochemical control of bimolecular thermochemical reactions in cholesteric liquid crystalline solvents

AUTHOR(S): Hiroka, Shingo; Yoshida, Takuro; Kansui, Hisao; Kunieda, Takehisa

Fac. Pharm. Sci., Kumamoto Univ., Kumamoto, 862, Japan CORPORATE SOURCE: Fac. Pharm. Sci., Kumamoto Univ., Kumamoto, 862, Japan
SOURCE: Tetrahedron Letters (1992), 33 (30), 4341-4
CODEN: Tetrahedron Letters (1992), 34 (4)
CODE

L12 ANSWER 10 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

PAGE 1-B

143878-94-8 CAPLUS
Cholest-5-en-3-ol (3.beta.)-, 4-methoxyphenyl 2,6-bis(decyloxy)-9,10-dihydro-9,10-ethanoanthracene-11,12-dicarboxylate, {3(9R,10R,11S,12S)}-(9CI) (CA INDEX NAME)

143878-95-9 CAPLUS Cholest-5-en-3-o1 (3.beta.)-, 2,6-bis(decyloxy)-9,10-dihydro-9,10-ethanoanthracene-11,12-dicarboxylate (2:1), {3(9R,10R,113,125}}- (9CI) (CA INDEX NAME)

L12 ANSWER 10 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

PAGE 1-A

PAGE 2-A

143878-93-7 CAPLUS
Cholest-5-en-3-ol (3.beta.)-, 4-methoxyphenyl 9,10-dihydro-2,6-bis(2-methoxypthoxy)-9,10-ethanoanthracene-11,12-dicarboxylate,
[3(9R,10R,11S,12S)]- (9CI) (CA INDEX NAME)

L12 ANSWER 10 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

PAGE 1-A

PAGE 2-A CH- (CH2) 3- CHMe2

143878-96-0 CAPLUS
Cholest-5-en-3-ol (3.beta.)-, [1,1'-bicyclohexyl]-4-yl
2,6-dibutoxy-9,10-dibydro-9,10-ethanoanthracene-11,12-dicarboxylate,
[3[9R,10R,11S,125(trans)]]- (9CI) (CA INDEX NAME)

PAGE 1-A

RN 143878-97-1 CAPLUS
CN Cholest-5-en-3-ol (3.beta.)-, [1,1'-bicyclohexyl]-4-yl
2,6-bis(decyloxy)-9,10-dihydro-9,10-ethanoanthracene-11,12-dicarboxylate,
[3[9R,10R,11S,12S(trans]]]- (9CI) (CA INDEX NAME)

L12 ANSWER 10 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



PAGE 2-A

RN 143879-00-9 CAPLUS
CN 9,10-Ethanoanthracene-11,12-dicarboxylic acid,
2,6-dibutoxy-9,10-dihydro-,
[1,1'-bicyclohexyl]-4-y1 4-methoxyphenyl ester,
[9,alpha.,10.alpha.,118*(trans),128*]- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 143879-01-0 CAPLUS
CN 9,10-Ethanoanthracene-11,12-dicarboxylic acid, 2,6-bis(decyloxy)-9,10dihydro-, [1,1'-bicyclohexyl]-4-yl 4-methoxyphenyl ester,
[9.alpha.,10.alpha.,115*(trans),125*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 143878-98-2 CAPLUS
CN 9,10-Ethanoanthracene-11,12-dicarboxylic acid,
2,6-dibutoxy-9,10-dihydro-,
bia{[1,1'-bicyclohexyl]-4-yl} ester,
[9.alpha.,10.alpha.,115'(trans),125'(
trans)]- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 143878-99-3 CAPLUS
Sy.10-Ethanoanthracene-11,12-dicarboxylic acid, 2,6-bis(decyloxy)-9,10-dihydro-, bis((1,1'-bicyclohexyl)-4-yl) ester,
[3.alpha.,10.alpha.,115*(trans),125*(trans)]- (9CI) (CA INDEX NAME)

Relative stereochemistry.

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

L12 ANSWER 10 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

RN 143955-14-0 CAPLUS
CN Cholest-5-en-3-ol (3.beta.)-, 4-methoxyphenyl 2,6-dibutoxy-9,10-dihydro9,10-ethanoanthracene-11,12-dicarboxylate, [3(9S,10S,11R,12R)]- (9CI)
(CA
INDEX NAME)

PAGE 1-A

PAGE 2-A

143955-15-1 CAPLUS Cholest-5-en-3-ol (3.beta.)-, 4-methoxyphenyl 2,6-dibutoxy-9,10-dihydro-9,10-ethanoanthracene-11,12-dicarboxylate, [3(9R,10R,11R,12R)]- (9CI) (CA

INDEX NAME)

PAGE 1-A

PAGE 2-A

143955-16-2 CAPLUS Cholest-5-en-3-ol (3.beta.)-, 4-methoxyphenyl 2,6-dibutoxy-9,10-dihydro-9,10-ethanoanthracene-11,12-dicarboxylate, [3(98,108,118,128)]- (9CI)

INDEX NAME)

L12 ANSWER 10 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

PAGE 1-B

-CHMe2

143955-18-4 CAPLUS Cholest-5-en-3-ol (3.beta.)-, 4-methoxyphenyl 9,10-dihydro-2,6-bis(2-methoxypthoxy)-9,10-ethanoanthracene-11,12-dicarboxylate, [3(9R,10R,11R,12R)]- (9CI) (CA INDEX NAME)

PAGE 1-B

L12 ANSWER 10 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

PAGE 1-A

PAGE 2-A

143955-17-3. CAPLUS
Cholest-5-en-3-ol (3.beta.)-, 4-methoxyphenyl 9,10-dihydro-2,6-bis(2-methoxyethoxy)-9,10-ethanoanthracene-11,12-dicarboxylate,
[3(9S,10S,11R,12R)]- (9CI) (CA INDEX NAME)

L12 ANSWER 10 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

143955-19-5 CAPLUS
Cholest-5-en-3-ol (3.beta.)-, 4-methoxyphenyl 9,10-dihydro-2,6-bis(2-methoxyethoxy)-9,10-ethanoanthracene-11,12-dicarboxylate,
[3(9S,10S,11S,12S)]- (9CI) (CA INDEX NAME)

PAGE 1-A сн₂-- сн₂-

PAGE 1-B

143955-20-8 CAPLUS Cholest-5-en-3-ol (3.beta.)-, 4-methoxyphenyl 2,6-bis(decyloxy)-9,10-dihydro-9,10-ethanoanthracene-11,12-dicarboxylate, [3(9S,10S,11R,12R)]-(9CI) (CA INDEX NAME)

143955-21-9 CAPLUS Cholest-5-en-3-o1 (3.beta.)-, 4-methoxyphenyl 2,6-bis(decyloxy)-9,10-dihydro-9,10-ethanoanthracene-11,12-dicarboxylate, [3(9R,10R,11R,12R)]-RN CN

RN 143955-22-0 CAPLUS
CN Cholest-5-en-3-ol (3.beta.)-, 4-methoxyphenyl 2,6-bis(decyloxy)-9,10-dihydro-9,10-ethanoanthracene-11,12-dicarboxylate, [3(9S,10S,11S,12S)]-(9CI) (CA INDEX NAME)

RN 143955-23-1 CAPLUS
CN Cholest-5-en-3-ol (3.beta.)-, 2,6-bis(decyloxy)-9,10-dihydro-9,10ethanoanthracene-11,12-dicarboxylate (2:1), [3(95,105,11R,12R)]- (9CI)
(CA INDEX NAME)

L12 ANSWER 10 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

PAGE 2-A

CH- (CH₂)₃-CHMe₂

RN 143955-25-3 CAPLUS
CN Cholest-5-en-3-ol (3.beta.)-, 2,6-bis(decyloxy)-9,10-dihydro-9,10ethanoanthracene-11,12-dicarboxylate (2:1), [3(9S,10S,11S,12S)]- (9CI)
(CA INDEX NAME)

L12 ANSWER 10 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

PAGE 1-A

PAGE 2-A CH- (CH₂)₃-CHMe₂

RN 143955-24-2 CAPLUS CN Cholest-5-en-3-ol (3.beta.)-, 2,6-bis(decyloxy)-9,10-dihydro-9,10ethanoanthracene-11,12-dicarboxylate (2:1), [3(9R,10R,11R,12R)]- (9CI) (CA INDEX NAME)

L12 ANSWER 10 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

PAGE 2-A

CH- (CH₂)₃-CHMe₂

Me

RN 143955-26-4 CAPLUS
CN Cholest-5-en-3-ol (3.beta.)-, [1,1'-bicyclohexyl]-4-yl
2,6-dibutoxy-9,10-dihydro-9,10-ethanoanthracene-11,12-dicarboxylate,
[3[9S,10S,11R,12R(trans)]]- (9CI) (CA INDEX NAME)

(Continued)

143955-27-5 CAPLUS
Cholest-5-en-3-ol (3.beta.)-, [1,1'-bicyclohexyl]-4-yl
2,6-dibutoxy-9,10-dihydro-9,10-ethanoanthracene-11,12-dicarboxylate,
[3[98,108,118,128(trans)]]- (9CI) (CA INDEX NAME)

L12 ANSWER 10 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

PAGE 2-A

143955-29-7 CAPLUS
Cholest-5-en-3-ol (3.beta.)-, {1,1'-bicyclohexyl}-4-yl
2,6-bis(dexyloxy)-9,10-dihydro-9,10-ethanoanthracene-11,12-dicarboxylate,
[3[95,105,11R,12R(trans)]]- (9CI) (CA INDEX NAME)

$$\bigcirc$$

PAGE 2-A

143955-28-6 CAPLUS
Cholest-5-en-3-ol (3.beta.)-, [1,1'-bicyclohexyl]-4-yl
2,6-dibutoxy-9,10-dihydro-9,10-ethanoanthracene-11,12-dicarboxylate,
[3[95,105,115,125[trans]]]- (9CI) (CA INDEX NAME)

L12 ANSWER 10 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

143955-30-0 CAPLUS Cholest-5-en-3-ol (3.beta.)-, [1,1'-bicyclohexyl]-4-yl 2,6-bis (dcyloxy)-9,10-dihydro-9,10-ethanoanthracene-11,12-dicarboxylate, [3[9R,10R,11R,12R(trans)]]- (9CI) (CA INDEX NAME)

143955-31-1 CAPLUS
Cholest-5-en-3-ol (3.beta.)-, [1,1'-bicyclohexyl]-4-yl
2,6-bia(deyloxy)-9,10-dihydro-9,10-ethanoanthracene-11,12-dicarboxylate,
[3[95,105,115,125(trans)]]- (9CI) (CA INDEX NAME)

RN 143955-32-2 CAPLUS
CN 9,10-Ethanoanthracene-11,12-dicarboxylic acid,
2,6-dibutoxy-9,10-dihydro-,
bis{[1,1'-bicyclohexyl]-4-yl} ester,
[9.alpha.,118*(trans),128*(
trans)]- (9CI) (CA INDEX NAME)

L12 ANSWER 10 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

PAGE 1-A

PAGE 1-C

L12 ANSWER 10 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

RN 143955-34-4 CAPLUS
CN 9,10-Ethanoanthracene-11,12-dicarboxylic acid,
2,6-dibutoxy-9,10-dihydro-,
[1,1-bicyclohexyl]-4-yl 4-methoxyphenyl ester,
[9.alpha.,10.alpha.,11R*(trans),12R*]- (9CI) (CA INDEX NAME)

RN 143955-35-5 CAPLUS

(N 9,10-Ethanoanthracene-11,12-dicarboxylic acid, 2,6-bis(decyloxy)-9,10-dihydro-, [1,1'-bicyclohexyl]-4-yl 4-methoxyphenyl ester, [9.alpha.,10.alpha.,11R*(trans),12R*]- (9CI) (CA INDEX NAME)

Relative stereochemistry.

L12 ANSWER 10 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

PAGE 2-A

RN 143955-36-6 CAPLUS
CN 9,10-Ethanoanthracene-11,12-dicarboxylic acid,
2,6-dibutoxy-9,10-dihydro-,
bis([1,1'-bicyclohexyl]-4-yl) ester,
[9.alpha.,10.alpha.,115'cia],128'ci
s)]- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 143955-37-7 CAPLUS
CN 9,10-Ethanoanthracene-11,12-dicarboxylic acid,
2,6-dibutoxy-9,10-dihydro-,
bis([1,1'-bicyclohexyl]-4-yl) ester,
[9.alpha.,10.alpha.,11R*(cis),12R*(cis),12R*(cis)]-(GCI) (CA INDEX NAME)

L12 ANSWER 11 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

36319-05-8 CAPLUS
9,10-Ethanoanthracene-11,12-dicarboxylic acid,
-dihydro-2,6-dimethoxy, (9.alpha.,10.alpha.,11R*,12R*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

134277-79-5 CAPLUS
9,10-Ethanoanthracene-11,12-dicarboxylic acid,
-dibutoxy-9,10-dihydro-,
(9.alpha.,10.alpha.,118*,128*)- (9CI) (CA INDEX NAME)

134277-80-8 CAPLUS
9,10-Ethanoanthracene-11,12-dicarboxylic acid, 9,10-dihydro-2,6-bis(2-methoxyethoxy)-, (9.alpha.,10.alpha.,118*,128*)- (9CI) (CA INDEX NAME)

134277-81-9 CAPLUS 9,10-Ethanoanthracene-11,12-dicarboxylic acid, 9,10-dihydro-2,6-bis(2-phenylethoxy)-, (9.alpha.,10.alpha.,118*,128*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

L12 ANSWER 11 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN GT

AB The uncatalyzed cycloaddns. of 2,6-dialkoxyanthracenes I (R = Me, Bu, MeoCH2CH2, PhCH2CH2) to cholesteric 1iq.-cryst. fumarates (E)-Rlo2CCH:CHCOR2 (R1 = cholesteryl; R2 = PhCH2CH2, Ph, 4-MeoC6H4, Me, Pr) serving both as dienophiles and media resulted in highly regioselective formation of the syn adducts II in up to 70% diastereomeric excess after sapon.

ACCESSION NUMBER: 1991:428844 CAPLUS
DOCUMENT NUMBER: 115:28844 Liquid crystalline dienophiles as regiochemical

1991:428844 CAPLUS 115:28844 Liquid crystalline dienophiles as regiochemical director in biomolecular Diels-Alder reactions Yamaguchi, Tatsuya; Yoshida, Takuro; Nagamatsu, Tomohisa; Kunieda, Takehisa; Honda, Takeshi; Hirobe, AUTHOR (S):

Masaaki Fac. Pharm. Sci., Kumamoto Univ., Kumamoto, 862, CORPORATE SOURCE:

Relative stereochemistry.

L12 ANSWER 11 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

RN 134356-32-4 CAPLUS
CN 9,10-Ethanoanthracene-11,12-dicarboxylic acid,
2,6-dibutoxy-9,10-dihydro-,
{9.alpha.,10.alpha.,11R*,12R*}- {9CI} (CA INDEX NAME)

Relative stereochemistry.

134356-33-5 CAPLUS
9,10-Ethanoanthracene-11,12-dicarboxylic acid, 9,10-dihydro-2,6-bis(2-methoxyethoxy)-, (9.alpha.,10.alpha.,11R*,12R*)- (9CI) (CA INDEX NAME)

134356-34-6 CAPLUS 9,10-Ethanoanthracene-11,12-dicarboxylic acid, 9,10-dihydro-2,6-bis{2-phenylethoxyl-, 9,.alpha.,10.alpha.,11R*,12R*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

L12 ANSWER 12 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN
AB Several members of a new class of water-sol. macrocycles with
well-defined, hydrophobic binding sites have been prepd. and their

well-defined, hydrophobic binding sites have been preped. and their binding properties. analyzed. These hosts are built up from ethenoanthracene units and exist in meso (C2h) and dl(D2) forms. The latter have been synthesized enantiomerically pure, the key step being a highly selective asym. Diels-Alder reaction. Several of these hosts display a strong and fairly general affinity for quaternary ammonlum compds, an effect ascribed to an ion-dipole attraction between the pos. charged guests and the electron-rich pi. systems of the hosts. In addn., neutral guests with electron-deficient .pi. systems are preferentially bound, suggesting the operation of favorable host-quest, donor-acceptor .pi.-stacking interactions. Preliminary studies with chiral guests reveal some enantiospecific binding, with preferences as large as 3:1 obsd.

ACCESSION NUMBER: 1989:438796 CAPLUS

DOCUMENT NUMBER: 111:38796

"Hydrophobic" binding of water-soluble guests by

111:38796 "Hydrophobic" binding of water-soluble guests by high-symmetry, chiral hosts. An electron-rich TITLE:

receptor

site with a general affinity for quaternary ammonium compounds and electron-deficient .pi. systems Pettl, Michael A.; Shepodd, Timothy J.; Barrans, Richard E., Jr.; Dougherty, Dennis A. Arnold and Mabel Beckman Lab. Chem. Synth., AUTHOR (S):

CORPORATE SOURCE: California

Inst. Technol., Pasadena, CA, 91125, USA Journal of the American Chemical Society (1988), 110(20), 6825-40 CODEN: JACSAT: ISSN: 0002-7863

SOURCE:

DOCUMENT TYPE: Journal

English CASREACT 111:38796 OTHER SOURCE (S): IT 116264-95-01

OTHER SOURCE(S):

CASREACT 111:38796

IT 1624-95-0P 116346-78-2P

RL: RCT (Reactant): SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or respent)

(prepn. and oxidn. and hydrolysis of)

RN 1626-95-0 CAPIUS

CN 9,10-Ethanoanthracene-11,12-dicarboxylic acid, 2,6-bis[[1,1-dimethylethyl] dimethylethyl] oxyl-9,10-dihydro-, bis[5-methyl-2-(1-methylethyl) cyclohexyl] ester,

[9x-[9.alpha.,10.alpha.,11x*(1s*,2x*,5s*),1

2x*(1s*,2x*,5s*)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L12 ANSWER 12 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN

(Continued) PAGE 1-A

PAGE 1-B

L12 ANSWER 12 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

PAGE 1-B

RN 116346-78-2 CAPLUS
SN 9,10-Ethanoanthracene-11,12-dicarboxylic acid, 2,6-bis[[{1,1-dimethylethylldimethylsilyl]oxy}-9,10-dihydro-, bis[5-methyl-2-(1-methylethyl)cyclohexyl] ester,
[9s-[9.alpha.,10.alpha.,11s-{11s-{11r.2s-{5r+1,1}}}-(2s-{11r.2s-{5r-1}}-(2s-{11r.2s-1}-(2s-{11r.2s-1}-(2s-{11r.2s-1}-(2s-{11r.2s-1}-(2s-{11r.2s-1}-(2s-{11r.2s-1}-(2s-{11r.2s-1}-(

Absolute stereochemistry.

L12 ANSWER 13 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN

AB In methoxybenzobicyclo[2.2.2]octen-2-one derivs. a change in the position of the MeO group causes a change in the direction of the transition

dipole

moment without much alteration in the .sigma.-electron distribution. The
effects of the change of the direction of the local chromophore on the
optical activity were studied and analyzed by the application of dynamic
and static coupling mechanisms. The optical activity is mainly produced
by .vector..mu.-.vector.m coupling and depends on the direction of the
local transition moments.

ACCESSION NUMBER: 1378:169387 CAPLUS
DOCUMENT NUMBER: 88:169387
TITLE: Optical activity in .beta..gamma.-unsaturated

TITLE: Optical activity in .beta..gamma.-unsaturated

Part 1. Effect of the direction of the electric transition dipole moment in the aromatic group in benzobicyclo[2.2.2]octen-2-one derivatives Hagishita, Sanji; Kuriyama, Kaoru Shionogi Res. Lab., Shionogi and Co. Ltd., Osaka, Jacon AUTHOR(S): CORPORATE SOURCE:

Shionogi Res. Lab., Shionogi and Co. Ltd., Osaka, Japan Journal of the Chemical Society, Perkin Transactions 2: Physical Organic Chemistry (1972-1999) (1977), (14), 1937-41 CODEN: JCPKBH; ISSN: 0300-9580 Journal SOURCE:

NAME)

RN 66289-18-7 CAPLUS
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid,
1,2,3,4-tetraphyto-6-methoxy9-oxo-, dimethyl ester, {1.alpha.,2.beta.,3.alpha.,4.alpha.}- (9CI) (CA

L12 ANSWER 14 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

L12 ANSWER 14 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN

AB The Diels-Alder reactions of several 2-methoxyanthracenes with tetracyanoethylene (TCNE), dimethyl acetylenedicarboxylate (DMAD), and maleic anhydride (HA) were examd. TCNE gave charge-transfer complexes, but not an addn. product in every case. HA gave one-to-one adducts with anthracenes, while DMAD afforded no adduct.

ACCESSION NUMBER: 1376:524992 CAPLUS

DOCUMENT NUMBER: 55:142892

TITLE: Pyridoxal model compounds. II. The Diels-Alder reaction of 9-substituted 2-methoxyanthracenes

AUTHOR(S): Inst. Phys. Chem. Res., Wako, Japan

SOURCE: Bulletin of the Chemical Society of Japan (1976), 49(4), 1163-4

CODEN BCSJA8; ISSN: 0009-2673

DOCUMENT TYPE: Journal LANGUAGE: English

IT 60626-33-9 60661-49-68P

RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of)

RN 60626-33-9 CAPLUS

0 9,10-Ethanoanthracene-11,12-dicarboxylic acid, 1-formyl-9,10-dihydro-2-methoxy-9-(2-methyl-4-(1-methylethyl)phenyl)- dimethyl ester, (9,alpha,.10.beta.,118*,128*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

Relative stereochemistry.

60661-49-6 CAPLUS
9,10-Ethanoanthracene-11,12-dicarboxylic acid, 1-formyl-9,10-dihydro-2-methoxy-9-[2-methyl-4-(1-methylethyl)phenyl]-, dimethyl ester,
(9.alpha.,10.beta.,11R*,12S*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

ANSWER 15 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN

AB Optically active C2-sym. 9, 10-dihydro-9, 10-ethanoanthracene (DEA) derivs.

Were prepd. and their abs. configurations detd. by kinetic resolution of
PhCH-MeOH with optically active DEA 11, 12-dicarboxylic acid chloride,
spectroscopic studies and chem. correlations. The rotational strengths
for the .alpha.— and p-band regions calcd. from the dipole-velocity
procedure in the .pi.-SCF approxn., rather than the point-dipole exciton
treatment, are in good agreement with expt. Although the rotational
strengths are mainly produced from coupling of local excitations, the
charge-transfer configurations cause inversion of the sequence of the
transition energy of the A and B combination in the excited

configurations
in certain cases. This is the most important factor in the inconsistency between exptl. and calcd. results based on the exciton approxn. in which it is assumed that there is no electron exchange between the 2 chromophores.

ACCESSION NUMBER: 1972:139860 CAPLUS
DOCUMENT NUMBER: 76:139860
TITLE:

TITLE:

19/2:13980

Optical activity of C2 symmetrical
9,10-dihydro-9,10-ethanoanthracenes
Hagishita, Sanji: Kuriyama, Kaoru
Shionogi Res. Lab., Shionogi and Co., Ltd., Osaka, AUTHOR(S): CORPORATE SOURCE:

SOURCE:

Japan Tetrahedron (1972), 28(6), 1435-67 CODEN: TETRAB; ISSN: 0040-4020 Journal

DOCUMENT TYPE: LANGUAGE: IT 36319-04-78

DOCUMENT TYPE: JOHENAL
LANGUAGE: English
English
17 36319-04-7P 36319-05-8P 36319-06-9P
36319-07-0P 36319-08-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 36319-04-7 CAPLUS
CN 9,10-Ethanoanthracene-11,12-dicarboxylic acid,
9,10-dihydro-2,6-dimethoxy, (9,alpha.,10.alpha.,115*,125*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 36319-05-8 CAPLUS
CN 9,10-Ethanoanthracene-11,12-dicarboxylic acid,
9,10-dihydro-2,6-dimethoxy, (9,alpha.,10.alpha.,11R*,12R*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 36319-06-9 CAPLUS
CN 9,10-Ethanoanthracene-11,12-dicarboxylic acid,
9,10-dihydro-2,6-dimethoxy, dimethyl ester, (9.alpha.,10.alpha.,115*,125*)- (9CI) (CA INDEX NAME)

(Continued)

Relative stereochemistry.

RN 36319-07-0 CAPLUS
CN 9,10-Ethanoanthracene-11,12-dicarboxylic acid,
9,10-dihydro-2,6-dimethoxy, dimethyl ester, (9.alpha.,10.alpha.,11R*,12R*)- (9CI) (CA INDEX NAME)

RN 36319-08-1 CAPLUS
CN 9,10-Ethanoanthracene-11,12-dicarboxylic acid,
9,10-dihydro-2,6-dimethoxy, (9,alpha.,10.alpha.,118*,128*)-(+)- (9CI) (CA INDEX NAME)

Rotation (+). Absolute stereochemistry unknown.

L12 ANSWER 16 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN

AB The Diels-Alder reaction of 1,7-, 2,7-, 2,6-, and

1,6-dihydroxynaphthalene
and 6-bromo-2-naphthol with maleic anhydride was investigated. All of
these 2-naphthol derivs, gave exo and endo adducts except for the
bromonaphthol, from which only an endo adduct was obtained. The
assignment of exo or endo configuration was based on lactone formation on
NaBH4 redn. (possible only from the exo isomer), comparison of NMR
spectra, and in some cases dipole moment measurements. The exo-endo
ratios of the formed adducts vary over a wide range. Title resolution
was

accomplished via the cinchonidine salts. The abs. configuration of the resolved compds. was detd. by applying the octant rule.

ACCESSION NUMBER: 1970:414534 CAPIUS

DOCUMENT NUMBER: 2,6,- and 1,6-dihydroxynaphthalene and 6-bromo-2-naphthol with maleic anhydride and the resolution of some derivatives of the adducts

AUTHOR(S): Takeda, Kenichi; Hagishita, Sanji; Sugiura, Michi; Kitahonoki, Keizo; Ban, Isoo; Miyazaki, Sadao; Kuriyama, Kaoru

CORPORATE SOURCE: Shionogi Res. Lab., Shionogi and Co. Ltd., Osaka, Japan

ORATE SOURCE: Shionogi Res. Lab., Shionogi and Co Japan CE: Tetrahedron (1970), 26(6), 1435-51 CODEN: TETRAB: ISSN: 0040-4020 JOURNAL UMGE: English 29038-00-4P 29038-11-7P 29073-46-9P 29073-48-1P 29073-55-0P 29073-57-2P 29073-64-1P 29073-10-79 29073-72-1P 29196-80-3P 29206-51-7P 31770-13-5P

SOURCE:

DOCUMENT TYPE: LANGUAGE:

31770-14-6P

RN 29038-11-7 CAPLUS
CN 1.4-Ethanonaphthalene-2,3-dicarboxylic acid,
1.alpha.,2.alpha.,4.
alpha.-tetrahydro-6-hydroxy-10-oxo-, dimethyl ester, (.+-.)- (8CI) (CA INDEX NAME)

29073-57-2 CAPLUS
1,4-Ethanonaphthalene-2,3-dicarboxylic acid,
7,4-tetrapdyco-6-methoxy10-oxo-, [1R-(1.alpha.,2.beta.,3.alpha.,4.alpha.)]- (9CI) (CA INDEX NAME

L12 ANSWER 16 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

RN 29073-46-9 CAPLUS
CN 1.4-Ethanonaphthalene-2,3-dicarboxylic acid,
1.alpha.,2.beta.,3.alpha.,4.a
lpha.-tetrahydro-6-methoxy-9-oxo-, (.+-.)- (8CI) (CA INDEX NAME)

RN 29073-48-1 CAPLUS
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid,
1.alpha.,2.alpha.,3.beta.,4.a
lpha.-tetrahydro-6-methoxy-10-oxo-, (.+-.)- (8CI) (CA INDEX NAME)

CO2H **F**.

RN 29073-55-0 CAPLUS
CN 1.4-Ethanonaphthalene-2,3-dicarboxylic acid,
1.alpha.,2.beta.,3.alpha.,4.a
lpha.-tetrahydro-10-hydroxy-6-methoxy-, (.+-.)- (8CI) (CA INDEX NAME)

29073-64-1 CAPLUS Cinchonidine, (18,28,38,4R)-(+)-1,2,3,4-tetrahydro-6-methoxy-9-oxo-1,4-ethanonaphthalene-2,3-dicarboxylate (1:1) (8CI) (CA INDEX NAME)

CM 1

CRN 47131-85-1 CMF C15 H14 O6

CO2H `со₂н

CM 2

CRN 485-71-2 CMF C19 H22 N2 O

Absolute stereochemistry.

RN 29073-71-0 CAPLUS
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid,
1.alpha.,2.beta.,3.beta.,4.al
pha.-tetrahydro-6-methoxy-9-oxo-, dimethyl ester, (.+-.)- (8CI) (CA
INDEX
NUMBERS | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 NAME)

L12 ANSWER 16 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

RN 31770-13-5 CAPLUS
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid,
1,2,3,4-terhaydro-6-methoxy9-oxo-, disedium salt, {15,25,35,4R}-{+}- {8CI} (CA INDEX NAME)

●2 Na

RN 31770-14-6 CAPLUS
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid,
1.alpha.,2.beta.,3.alpha.,4.a
lpha.-tetrahydro-6-methoxy-10-oxo-, (.+-.)- (8CI) (CA INDEX NAME)

L12 ANSWER 16 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

RN 29073-72-1 CAPLUS
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid,
1.alpha.,2.alpha.,3.alpha.,4.
alpha.tetrahydro-6-methoxy-10-oxo-, dimethyl ester, (.+-.)- (8CI) (CA INDEX NAME)

RN 29196-80-3 CAPLUS
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid,
1.alpha.,2.alpha.,3.alpha.,4.
alpha.-tetrahydro-6-methoxy-9-oxo-, dimethyl ester, (.+-.)- (8CI) (CA INDEX NAME)

RN 29206-51-7 CAPLUS
CN 1,4-Ethanonaphthalene-2,3-dicarboxylic acid,
1.alpha.,2.alpha.,3.alpha.,4.
alpha.-tetrahydro-6-hydroxy-9-oxo-, dimethyl ester, (.+-.)- (8CI) (CA INDEX NAME)

=> logoff y COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION

81.75 FULL ESTIMATED COST 539.62

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL ENTRY SESSION

CA SUBSCRIBER PRICE -11.72 -10.42

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